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# Crystal structure of $\text{Al}_{45}\text{Cr}_7\text{C}_{0.32}$

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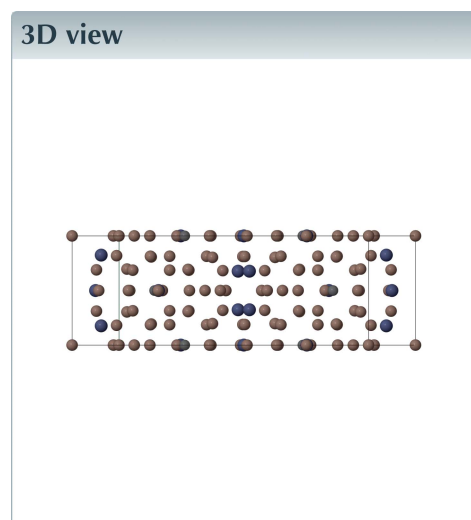
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Structural data: full structural data are available from [iucrdata.iucr.org](http://iucrdata.iucr.org)

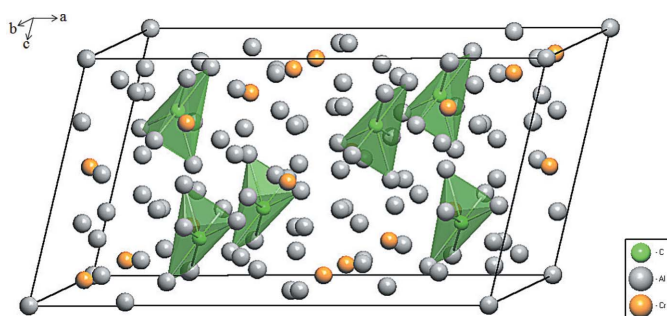
During a high-pressure sintering (HPS) process of a stoichiometric  $\text{Al}_7\text{Cr}$  mixture, the ternary phase  $\text{Al}_{45}\text{Cr}_7\text{C}_{0.32}$  (pentatetraconta-aluminium heptachromium carbide) was obtained serendipitously. The C atom (occupancy 0.32) is irregularly surrounded by six Al atoms.



## Structure description

Phase formation of a quasicrystalline phase in an Al–Cr alloy by ion irradiation of an amorphous film was reported by Lilienfeld *et al.* (1986). The structure of the binary phase  $\text{Al}_{45}\text{Cr}_7$  ( $\theta$ -Al<sub>7</sub>Cr) phase was determined by Cooper (1960) in the space group  $C2/m$ , with  $a = 25.196$ ,  $b = 7.574$ ,  $c = 10.949$  Å,  $\beta = 128^\circ 43'$ . This phase is isotypic with  $\text{Al}_{45}\text{V}_7$ . In a redetermination of  $\theta$ -Al<sub>7</sub>Cr, He *et al.* (2006) used a different unit-cell setting with  $a = 20.595$ ,  $b = 7.574$ ,  $c = 10.949$  Å,  $\beta = 107.34^\circ$ . During a project aimed at formation of quasicrystalline material in the Al–Cr system under high-pressure conditions, we obtained the title compound and learned that light atoms can be incorporated into the  $\text{Al}_{45}\text{Cr}_7$  host structure. We attribute the slight increase in the unit-cell lengths and the decrease in the monoclinic angle in comparison with the values of the binary phase reported by He *et al.* (2006) ( $\Delta a = 0.028$  Å,  $\Delta b = 0.016$  Å,  $\Delta c = 0.0136$  Å,  $\Delta\beta = -0.03^\circ$ ) to the presence of partially occupied light atoms that must have been diffused into the crystal structure during the HPS process, or were present as impurities in the employed metals. In principle, the light atoms could be boron, nitrogen (from the BN crucible), or carbon (from the graphite liner). In fact, we found that the educts were contaminated by small amounts of carbon (see Supplementary information).

The asymmetric unit of  $\text{Al}_{45}\text{Cr}_7\text{C}_{0.32}$  comprises of sixteen Al, three Cr and one partially occupied C sites (occupancy 0.32). Since the host structure has been described in detail (Cooper, 1960; He *et al.*, 2006), we discuss here only the role of the additional carbon atom in  $\text{Al}_{45}\text{Cr}_7\text{C}_{0.32}$ . The position of the C1 atom in the crystal structure can be seen in Fig. 1. It is located on a site with symmetry  $m$  (Wyckoff position  $4i$ ) and is connected to six

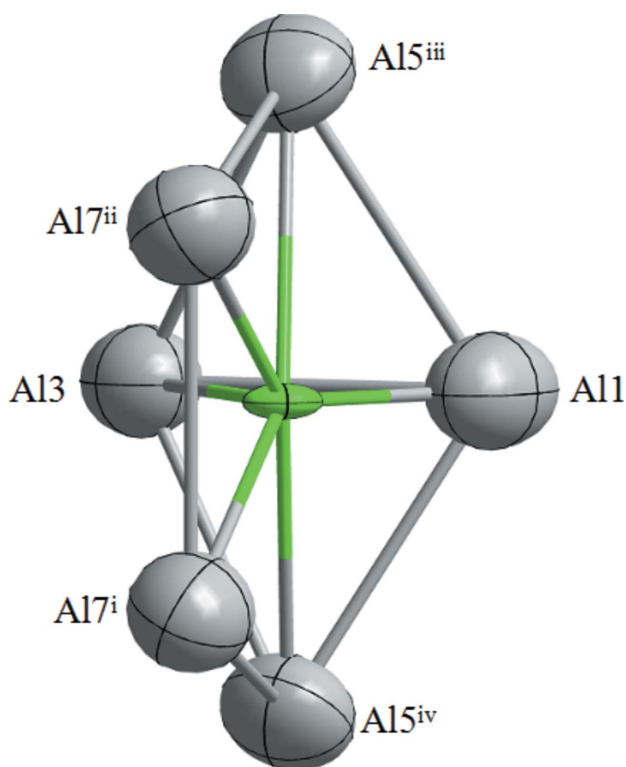


**Figure 1**  
The crystal structure of  $\text{Al}_{45}\text{Cr}_7\text{C}_{0.32}$ . The  $\text{Al}_6$  polyhedra around C1 atoms are emphasized.

Al atoms that form an irregular polyhedron (Fig. 2). The distances between C1 and Al1, Al3, Al5 and Al7 are 1.878 (16), 2.351 (16), 2.497 (6) and 2.378 (13) Å, respectively.

### Synthesis and crystallization

The elements Al (indicated purity 99.8%) and Cr (indicated purity 99.95%) were mixed in the stoichiometric ratio of 7:1 and initially ground in an agate mortar. The blended powders were then placed into a grinding tool with a diameter of 9.6 mm and pressed into a tablet at about 3.5 MPa slowly and continuously for about 5 minutes. A cylindrical block 9.6 mm



**Figure 2**  
The coordination sphere of the underoccupied C1 atom in detail. Displacement ellipsoids are given at the 99% probability level. [Symmetry codes: (i)  $-x + \frac{1}{2}, -y + \frac{1}{2}, -z + 1$ ; (ii)  $-x + \frac{1}{2}, y + \frac{1}{2}, -z + 1$ ; (iii)  $-x + \frac{1}{2}, -y + \frac{3}{2}, -z + 1$ ; (iv)  $-x + \frac{1}{2}, y - \frac{1}{2}, -z + 1$ ]

**Table 1**  
Experimental details.

Crystal data	
Chemical formula	$\text{Al}_{45}\text{Cr}_7\text{C}_{0.32}$
$M_r$	1581.95
Crystal system, space group	Monoclinic, $C2/m$
Temperature (K)	293
$a, b, c$ (Å)	20.623 (2), 7.5900 (9), 10.9626 (13)
$\beta$ (°)	107.310 (3)
$V$ (Å <sup>3</sup> )	1638.2 (3)
$Z$	2
Radiation type	Mo $K\alpha$
$\mu$ (mm <sup>-1</sup> )	3.46
Crystal size (mm)	0.05 × 0.04 × 0.02
Data collection	
Diffractometer	Bruker APEXII Photon 100 CMOS
Absorption correction	Multi-scan ( <i>SADABS</i> ; Bruker, 2015)
$T_{\text{min}}, T_{\text{max}}$	0.553, 0.746
No. of measured, independent and observed [ $I > 2\sigma(I)$ ] reflections	9513, 2191, 1903
$R_{\text{int}}$	0.038
$(\sin \theta/\lambda)_{\text{max}}$ (Å <sup>-1</sup> )	0.669
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.027, 0.060, 1.03
No. of reflections	2191
No. of parameters	142
No. of restraints	6
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å <sup>-3</sup> )	0.54, -0.71

Computer programs: *APEX3* and *SAINT* (Bruker, 2015), *SHELXT* (Sheldrick, 2015a), *SHELXL2014/7* (Sheldrick, 2015b), *DIAMOND* (Brandenburg & Putz, 2017) and *publCIF* (Westrip, 2010).

in diameter and 10.0 mm in height was obtained without any defects such as cracks or deformations. The cylindrical block was then inserted into a six-anvil high-pressure apparatus for HPS experiments, pressurized up to 5 GPa and heated to 1183 K for 30 minutes, cooled to 1033 K and held at that temperature for 2 h, and then rapidly cooled down to room temperature. A fragment  $0.05 \times 0.04 \times 0.02 \text{ mm}^3$  in size was selected and mounted on a glass fiber for single-crystal X-ray diffraction measurements.

### Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. After consideration of all atoms in the  $\text{Al}_{45}\text{Cr}_7$  structure, we found significant remaining electron density ( $2.1 \text{ e}^- \text{ Å}^3$ ) that was modelled as a carbon atom with partial occupancy. The site occupation factor was refined freely and converged at 0.160 (11). The C atom was treated with an ISOR command to get a physically reasonable shape. The remaining maximum and minimum electron densities are located 0.88 Å from atom Al6 and 0.48 Å from atom Cr1, respectively.

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**References**

- Brandenburg, K. & Putz, H. (2017). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
- Bruker (2015). *APEX3*, *SAINTE* and *SADABS*, Bruker AXS Inc. Madison, Wisconsin, USA, 2008.
- Cooper, M. J. (1960). *Acta Cryst.* **13**, 257–263.
- He, Z. B., Zou, B. S. & Kuo, K. H. (2006). *J. Alloys Compd.* **417**, L4–L8.
- Lilienfeld, D. A., Nastasi, M., Johnson, H. H., Ast, D. G. & Mayer, W. (1986). *J. Mater. Res.* **1**, 237–242.
- Sheldrick, G. M. (2015a). *Acta Cryst.* **A71**, 3–8.
- Sheldrick, G. M. (2015b). *Acta Cryst.* **C71**, 3–8.
- Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

## full crystallographic data

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Crystal structure of  $\text{Al}_{45}\text{Cr}_7\text{C}_{0.32}$ 

Cong Liu and Changzeng Fan

## Pentatetraconta-aluminium heptachromium carbide

*Crystal data*

$\text{C}_{0.32}\text{Al}_{45}\text{Cr}_7$	$F(000) = 1510$
$M_r = 1581.95$	$D_x = 3.207 \text{ Mg m}^{-3}$
Monoclinic, $C2/m$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
$a = 20.623 (2) \text{ \AA}$	Cell parameters from 1903 reflections
$b = 7.5900 (9) \text{ \AA}$	$\theta = 2.9\text{--}28.4^\circ$
$c = 10.9626 (13) \text{ \AA}$	$\mu = 3.46 \text{ mm}^{-1}$
$\beta = 107.310 (3)^\circ$	$T = 293 \text{ K}$
$V = 1638.2 (3) \text{ \AA}^3$	Grain, metallic
$Z = 2$	$0.05 \times 0.04 \times 0.02 \text{ mm}$

*Data collection*

Bruker APEXII Photon 100 CMOS diffractometer	2191 independent reflections
phi and $\omega$ scans	1903 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan ( <i>SADABS</i> ; Bruker, 2015)	$R_{\text{int}} = 0.038$
$T_{\text{min}} = 0.553$ , $T_{\text{max}} = 0.746$	$\theta_{\text{max}} = 28.4^\circ$ , $\theta_{\text{min}} = 2.9^\circ$
9513 measured reflections	$h = -27 \rightarrow 27$
	$k = -10 \rightarrow 9$
	$l = -14 \rightarrow 14$

*Refinement*

Refinement on $F^2$	6 restraints
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0188P)^2 + 4.4834P]$
$R[F^2 > 2\sigma(F^2)] = 0.027$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.060$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$S = 1.02$	$\Delta\rho_{\text{max}} = 0.54 \text{ e \AA}^{-3}$
2191 reflections	$\Delta\rho_{\text{min}} = -0.71 \text{ e \AA}^{-3}$
142 parameters	

*Special details*

**Geometry.** All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Al1	0.09059 (5)	0.5000	0.34230 (10)	0.0142 (2)	
Cr1	0.0000	0.5000	0.5000	0.00839 (15)	

C1	0.1632 (8)	0.5000	0.2718 (16)	0.003 (5)	0.160 (11)
Al2	0.12849 (5)	0.5000	0.61192 (9)	0.0116 (2)	
Cr2	0.25029 (2)	0.5000	0.73869 (5)	0.00844 (12)	
Al3	0.22392 (5)	0.5000	0.49039 (9)	0.0115 (2)	
Cr3	0.58523 (2)	0.32368 (5)	0.91792 (3)	0.00790 (9)	
Al4	0.29353 (3)	0.68643 (9)	0.36573 (7)	0.01277 (15)	
Al5	0.33511 (4)	0.69296 (10)	0.64551 (7)	0.01313 (15)	
Al6	0.37439 (4)	0.5000	0.86551 (9)	0.00862 (19)	
Al7	0.31030 (3)	0.18598 (10)	0.88132 (7)	0.01337 (16)	
Al8	0.29273 (5)	0.5000	1.01491 (9)	0.0114 (2)	
Al9	0.5000	0.5000	1.0000	0.0076 (3)	
Al10	0.45400 (3)	0.19674 (9)	0.87763 (6)	0.01182 (15)	
Al11	0.47798 (5)	0.5000	0.74372 (9)	0.0109 (2)	
Al12	0.43072 (3)	0.31858 (9)	0.51014 (7)	0.01300 (16)	
Al13	0.53571 (3)	0.18856 (9)	0.70481 (6)	0.01140 (15)	
Al14	0.61492 (5)	0.5000	0.72906 (9)	0.0113 (2)	
Al15	0.68150 (3)	0.18638 (9)	0.85428 (6)	0.01101 (15)	
Al16	0.58033 (5)	0.0000	0.93926 (9)	0.0111 (2)	

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Al1	0.0138 (5)	0.0110 (5)	0.0149 (5)	0.000	0.0000 (4)	0.000
Cr1	0.0091 (3)	0.0064 (4)	0.0092 (3)	0.000	0.0020 (3)	0.000
C1	0.005 (6)	0.001 (6)	0.003 (6)	0.000	0.001 (4)	0.000
Al2	0.0094 (4)	0.0112 (5)	0.0137 (5)	0.000	0.0027 (4)	0.000
Cr2	0.0080 (2)	0.0083 (3)	0.0091 (2)	0.000	0.00262 (19)	0.000
Al3	0.0122 (4)	0.0102 (5)	0.0126 (5)	0.000	0.0043 (4)	0.000
Cr3	0.00858 (17)	0.00604 (19)	0.00929 (17)	-0.00005 (13)	0.00299 (13)	-0.00042 (13)
Al4	0.0141 (3)	0.0102 (4)	0.0153 (3)	0.0005 (3)	0.0065 (3)	0.0020 (3)
Al5	0.0149 (3)	0.0113 (4)	0.0140 (3)	-0.0015 (3)	0.0055 (3)	0.0013 (3)
Al6	0.0078 (4)	0.0077 (5)	0.0097 (4)	0.000	0.0016 (3)	0.000
Al7	0.0132 (3)	0.0118 (4)	0.0145 (3)	0.0005 (3)	0.0030 (3)	0.0011 (3)
Al8	0.0110 (4)	0.0088 (5)	0.0139 (5)	0.000	0.0031 (4)	0.000
Al9	0.0067 (6)	0.0065 (7)	0.0100 (6)	0.000	0.0031 (5)	0.000
Al10	0.0140 (3)	0.0091 (4)	0.0133 (3)	-0.0007 (3)	0.0056 (3)	-0.0007 (3)
Al11	0.0131 (4)	0.0083 (5)	0.0116 (4)	0.000	0.0041 (4)	0.000
Al12	0.0137 (3)	0.0114 (4)	0.0130 (3)	0.0011 (3)	0.0026 (3)	-0.0006 (3)
Al13	0.0130 (3)	0.0090 (4)	0.0114 (3)	-0.0002 (3)	0.0024 (3)	-0.0015 (3)
Al14	0.0137 (5)	0.0080 (5)	0.0131 (5)	0.000	0.0050 (4)	0.000
Al15	0.0113 (3)	0.0088 (4)	0.0139 (3)	0.0006 (3)	0.0052 (3)	-0.0007 (3)
Al16	0.0146 (5)	0.0060 (5)	0.0135 (5)	0.000	0.0054 (4)	0.000

*Geometric parameters (Å, °)*

Al1—C1	1.878 (16)	Al6—Al7 <sup>viii</sup>	2.7557 (9)
Al1—Al3	2.7458 (14)	Al6—Al7	2.7557 (9)
Al1—Al10 <sup>i</sup>	2.7512 (11)	Al6—Al10 <sup>viii</sup>	2.8073 (9)

Al1—Al10 <sup>ii</sup>	2.7512 (11)	Al6—Al10	2.8073 (9)
Al1—Al5 <sup>iii</sup>	2.7703 (9)	Al6—Al11	2.8362 (13)
Al1—Al5 <sup>iv</sup>	2.7703 (9)	Al7—C1 <sup>i</sup>	2.378 (13)
Al1—Al2	2.8235 (14)	Al7—Al15 <sup>vii</sup>	2.7592 (10)
Al1—Al13 <sup>i</sup>	2.8807 (11)	Al7—Cr3 <sup>x</sup>	2.7848 (8)
Al1—Al13 <sup>ii</sup>	2.8807 (11)	Al7—Al7 <sup>xii</sup>	2.8232 (15)
Al1—Cr1	2.8983 (11)	Al7—Al15 <sup>x</sup>	2.8528 (10)
Cr1—Al2	2.5674 (10)	Al7—Al8	2.8762 (9)
Cr1—Al2 <sup>v</sup>	2.5675 (10)	Al7—Al16 <sup>xiii</sup>	2.8824 (11)
Cr1—Al13 <sup>i</sup>	2.5783 (7)	Al7—Al4 <sup>iv</sup>	2.9101 (10)
Cr1—Al13 <sup>vi</sup>	2.5783 (7)	Al7—Al5 <sup>viii</sup>	2.9284 (10)
Cr1—Al13 <sup>vii</sup>	2.5783 (7)	Al7—Al10	2.9768 (10)
Cr1—Al13 <sup>ii</sup>	2.5783 (7)	Al8—Al15 <sup>ix</sup>	2.7480 (9)
Cr1—Al12 <sup>vii</sup>	2.8275 (8)	Al8—Al15 <sup>x</sup>	2.7480 (9)
Cr1—Al12 <sup>ii</sup>	2.8275 (8)	Al8—Cr3 <sup>ix</sup>	2.7503 (9)
Cr1—Al12 <sup>vi</sup>	2.8275 (7)	Al8—Cr3 <sup>x</sup>	2.7503 (9)
Cr1—Al12 <sup>i</sup>	2.8275 (7)	Al8—Al15 <sup>vii</sup>	2.8213 (11)
Cr1—Al1 <sup>v</sup>	2.8983 (11)	Al8—Al15 <sup>vi</sup>	2.8213 (11)
C1—Al1	1.878 (16)	Al8—Al7 <sup>viii</sup>	2.8761 (9)
C1—Al3	2.351 (16)	Al8—Al14 <sup>ix</sup>	2.8851 (14)
C1—Al7 <sup>i</sup>	2.378 (13)	Al9—Al6 <sup>ix</sup>	2.5712 (9)
C1—Al7 <sup>ii</sup>	2.378 (13)	Al9—Cr3 <sup>viii</sup>	2.5752 (4)
C1—Al5 <sup>iii</sup>	2.497 (6)	Al9—Cr3 <sup>x</sup>	2.5752 (4)
C1—Al5 <sup>iv</sup>	2.497 (6)	Al9—Cr3 <sup>ix</sup>	2.5752 (4)
Al2—Cr2	2.4827 (11)	Al9—Al10	2.6908 (7)
Al2—Al3	2.6849 (13)	Al9—Al10 <sup>ix</sup>	2.6908 (7)
Al2—Al13 <sup>vii</sup>	2.8116 (11)	Al9—Al10 <sup>viii</sup>	2.6908 (7)
Al2—Al13 <sup>vi</sup>	2.8116 (11)	Al9—Al10 <sup>x</sup>	2.6908 (7)
Al2—Al4 <sup>iii</sup>	2.8419 (9)	Al9—Al11 <sup>ix</sup>	2.7093 (10)
Al2—Al4 <sup>iv</sup>	2.8419 (9)	Al9—Al11	2.7093 (10)
Al2—Al12 <sup>i</sup>	2.8558 (9)	Al10—Al1 <sup>i</sup>	2.7512 (11)
Al2—Al12 <sup>ii</sup>	2.8558 (9)	Al10—Al16 <sup>xiii</sup>	2.7579 (11)
Al2—Al15 <sup>vi</sup>	2.9201 (11)	Al10—Cr3 <sup>x</sup>	2.7722 (8)
Al2—Al15 <sup>vii</sup>	2.9201 (11)	Al10—Al10 <sup>x</sup>	2.7873 (14)
Cr2—Al6	2.5230 (11)	Al10—Al11	2.8513 (9)
Cr2—Al15 <sup>vii</sup>	2.5863 (8)	Al10—Al13	2.8866 (10)
Cr2—Al15 <sup>vi</sup>	2.5863 (8)	Al10—Al16	2.9028 (11)
Cr2—Al3	2.6123 (11)	Al10—Al10 <sup>xii</sup>	2.9864 (15)
Cr2—Al4 <sup>iv</sup>	2.6787 (8)	Al11—Al13	2.7366 (9)
Cr2—Al4 <sup>iii</sup>	2.6787 (8)	Al11—Al13 <sup>viii</sup>	2.7366 (9)
Cr2—Al5	2.7040 (8)	Al11—Cr3 <sup>viii</sup>	2.7958 (9)
Cr2—Al5 <sup>viii</sup>	2.7040 (8)	Al11—Al12	2.8139 (11)
Cr2—Al8	2.8910 (11)	Al11—Al12 <sup>viii</sup>	2.8139 (11)
Cr2—Al7 <sup>viii</sup>	2.9165 (8)	Al11—Al10 <sup>viii</sup>	2.8514 (9)
Cr2—Al7	2.9165 (8)	Al11—Al14	2.8758 (14)
Al3—Al4	2.6642 (11)	Al12—Al13	2.7326 (10)
Al3—Al4 <sup>viii</sup>	2.6642 (11)	Al12—Al12 <sup>viii</sup>	2.7539 (15)
Al3—Al5	2.8240 (11)	Al12—Al5 <sup>viii</sup>	2.7998 (10)

Al3—Al5 <sup>viii</sup>	2.8240 (11)	Al12—Al4 <sup>viii</sup>	2.8013 (10)
Al3—Al5 <sup>iv</sup>	2.8378 (9)	Al12—Al13 <sup>xiv</sup>	2.8242 (10)
Al3—Al5 <sup>iii</sup>	2.8378 (9)	Al12—Cr1 <sup>xv</sup>	2.8275 (7)
Al3—Al4 <sup>iii</sup>	2.9359 (9)	Al12—Al2 <sup>i</sup>	2.8559 (9)
Al3—Al4 <sup>iv</sup>	2.9359 (9)	Al12—Al14 <sup>xi</sup>	2.8617 (11)
Cr3—Al16	2.4727 (5)	Al12—Al12 <sup>xiv</sup>	2.9313 (14)
Cr3—Al13	2.4765 (8)	Al13—Cr1 <sup>xv</sup>	2.5784 (7)
Cr3—Al15	2.5176 (8)	Al13—Al2 <sup>xv</sup>	2.8117 (11)
Cr3—Al9	2.5752 (4)	Al13—Al12 <sup>xiv</sup>	2.8243 (10)
Cr3—Al6 <sup>ix</sup>	2.6352 (9)	Al13—Al14	2.8404 (9)
Cr3—Cr3 <sup>viii</sup>	2.6766 (8)	Al13—Al16	2.8448 (11)
Cr3—Al14	2.6845 (9)	Al13—Al13 <sup>xii</sup>	2.8623 (14)
Cr3—Al8 <sup>ix</sup>	2.7503 (9)	Al13—Al1 <sup>i</sup>	2.8806 (11)
Cr3—Al10 <sup>x</sup>	2.7722 (8)	Al13—Al15	2.9653 (10)
Cr3—Al10	2.7815 (8)	Al14—Cr3 <sup>viii</sup>	2.6844 (9)
Cr3—Al7 <sup>x</sup>	2.7848 (8)	Al14—Al4 <sup>xiv</sup>	2.7955 (11)
Cr3—Al11	2.7958 (9)	Al14—Al4 <sup>xi</sup>	2.7955 (11)
Al4—Cr2 <sup>iii</sup>	2.6787 (8)	Al14—Al13 <sup>viii</sup>	2.8404 (9)
Al4—Al5 <sup>iii</sup>	2.7743 (10)	Al14—Al12 <sup>xiv</sup>	2.8617 (11)
Al4—Al15 <sup>xi</sup>	2.7844 (10)	Al14—Al12 <sup>xi</sup>	2.8617 (11)
Al4—Al14 <sup>xi</sup>	2.7955 (11)	Al14—Al15	2.8835 (9)
Al4—Al12 <sup>viii</sup>	2.8012 (10)	Al14—Al15 <sup>viii</sup>	2.8835 (9)
Al4—Al4 <sup>viii</sup>	2.8300 (15)	Al14—Al8 <sup>ix</sup>	2.8851 (14)
Al4—Al2 <sup>iii</sup>	2.8419 (9)	Al15—Cr2 <sup>xv</sup>	2.5863 (8)
Al4—Al7 <sup>ii</sup>	2.9101 (10)	Al15—Al8 <sup>ix</sup>	2.7480 (9)
Al4—Al5	2.9292 (10)	Al15—Al7 <sup>xvi</sup>	2.7592 (10)
Al4—Al3 <sup>iii</sup>	2.9359 (9)	Al15—Al4 <sup>xi</sup>	2.7844 (10)
Al5—C1 <sup>iii</sup>	2.497 (6)	Al15—Al8 <sup>xv</sup>	2.8214 (11)
Al5—Al6	2.7304 (10)	Al15—Al15 <sup>xii</sup>	2.8293 (14)
Al5—Al1 <sup>iii</sup>	2.7704 (9)	Al15—Al7 <sup>x</sup>	2.8528 (10)
Al5—Al4 <sup>iii</sup>	2.7742 (10)	Al15—Al16	2.8947 (11)
Al5—Al12 <sup>viii</sup>	2.7998 (10)	Al15—Al2 <sup>xv</sup>	2.9201 (11)
Al5—Al3 <sup>iii</sup>	2.8378 (9)	Al16—Cr3 <sup>xii</sup>	2.4727 (5)
Al5—Al7 <sup>viii</sup>	2.9285 (10)	Al16—Al10 <sup>x</sup>	2.7579 (11)
Al5—Al5 <sup>viii</sup>	2.9291 (15)	Al16—Al10 <sup>xiii</sup>	2.7579 (11)
Al6—Al9	2.5712 (9)	Al16—Al13 <sup>xii</sup>	2.8448 (11)
Al6—Cr3 <sup>ix</sup>	2.6352 (9)	Al16—Al7 <sup>x</sup>	2.8824 (11)
Al6—Cr3 <sup>x</sup>	2.6352 (9)	Al16—Al7 <sup>xiii</sup>	2.8824 (11)
Al6—Al8	2.6757 (13)	Al16—Al15 <sup>xii</sup>	2.8946 (11)
Al6—Al5 <sup>viii</sup>	2.7304 (11)	Al16—Al10 <sup>xii</sup>	2.9028 (11)
C1—Al1—Al3	57.5 (5)	Al15 <sup>x</sup> —Al7—Al16 <sup>xiii</sup>	60.62 (3)
C1—Al1—Al10 <sup>i</sup>	74.8 (4)	Al8—Al7—Al16 <sup>xiii</sup>	104.47 (3)
Al3—Al1—Al10 <sup>i</sup>	122.20 (4)	C1 <sup>i</sup> —Al7—Al4 <sup>iv</sup>	66.7 (4)
C1—Al1—Al10 <sup>ii</sup>	74.8 (4)	Al6—Al7—Al4 <sup>iv</sup>	100.04 (3)
Al3—Al1—Al10 <sup>ii</sup>	122.20 (4)	Al15 <sup>vii</sup> —Al7—Al4 <sup>iv</sup>	58.76 (2)
Al10 <sup>i</sup> —Al1—Al10 <sup>ii</sup>	65.74 (4)	Cr3 <sup>x</sup> —Al7—Al4 <sup>iv</sup>	156.49 (3)
C1—Al1—Al5 <sup>iii</sup>	61.49 (15)	Al7 <sup>xii</sup> —Al7—Al4 <sup>iv</sup>	90.07 (2)

Al3—Al1—Al5 <sup>iii</sup>	61.92 (2)	Al15 <sup>x</sup> —Al7—Al4 <sup>iv</sup>	138.62 (3)
Al10 <sup>i</sup> —Al1—Al5 <sup>iii</sup>	122.32 (4)	Al8—Al7—Al4 <sup>iv</sup>	107.67 (3)
Al10 <sup>ii</sup> —Al1—Al5 <sup>iii</sup>	67.76 (2)	Al16 <sup>xiii</sup> —Al7—Al4 <sup>iv</sup>	147.71 (3)
C1—Al1—Al5 <sup>iv</sup>	61.49 (15)	C1 <sup>i</sup> —Al7—Cr2	104.9 (3)
Al3—Al1—Al5 <sup>iv</sup>	61.92 (2)	Al6—Al7—Cr2	52.73 (2)
Al10 <sup>i</sup> —Al1—Al5 <sup>iv</sup>	67.76 (2)	Al15 <sup>vii</sup> —Al7—Cr2	54.13 (2)
Al10 <sup>ii</sup> —Al1—Al5 <sup>iv</sup>	122.32 (4)	Cr3 <sup>x</sup> —Al7—Cr2	102.83 (3)
Al5 <sup>iii</sup> —Al1—Al5 <sup>iv</sup>	114.53 (5)	Al7 <sup>xii</sup> —Al7—Cr2	144.809 (17)
C1—Al1—Al2	115.1 (5)	Al15 <sup>x</sup> —Al7—Cr2	115.55 (3)
Al3—Al1—Al2	57.62 (3)	Al8—Al7—Cr2	59.87 (3)
Al10 <sup>i</sup> —Al1—Al2	146.47 (2)	Al16 <sup>xiii</sup> —Al7—Cr2	152.52 (3)
Al10 <sup>ii</sup> —Al1—Al2	146.47 (2)	Al4 <sup>iv</sup> —Al7—Cr2	54.74 (2)
Al5 <sup>iii</sup> —Al1—Al2	88.43 (3)	C1 <sup>i</sup> —Al7—Al5 <sup>viii</sup>	55.0 (2)
Al5 <sup>iv</sup> —Al1—Al2	88.43 (3)	Al6—Al7—Al5 <sup>viii</sup>	57.32 (3)
C1—Al1—Al13 <sup>i</sup>	135.6 (4)	Al15 <sup>vii</sup> —Al7—Al5 <sup>viii</sup>	102.15 (3)
Al3—Al1—Al13 <sup>i</sup>	143.03 (3)	Cr3 <sup>x</sup> —Al7—Al5 <sup>viii</sup>	106.42 (3)
Al10 <sup>i</sup> —Al1—Al13 <sup>i</sup>	61.62 (3)	Al7 <sup>xii</sup> —Al7—Al5 <sup>viii</sup>	108.29 (2)
Al10 <sup>ii</sup> —Al1—Al13 <sup>i</sup>	93.67 (4)	Al15 <sup>x</sup> —Al7—Al5 <sup>viii</sup>	157.44 (3)
Al5 <sup>iii</sup> —Al1—Al13 <sup>i</sup>	152.15 (3)	Al8—Al7—Al5 <sup>viii</sup>	105.73 (3)
Al5 <sup>iv</sup> —Al1—Al13 <sup>i</sup>	92.77 (2)	Al16 <sup>xiii</sup> —Al7—Al5 <sup>viii</sup>	116.70 (3)
Al2—Al1—Al13 <sup>i</sup>	98.14 (4)	Al4 <sup>iv</sup> —Al7—Al5 <sup>viii</sup>	56.74 (2)
C1—Al1—Al13 <sup>ii</sup>	135.6 (4)	Cr2—Al7—Al5 <sup>viii</sup>	55.11 (2)
Al3—Al1—Al13 <sup>ii</sup>	143.03 (3)	C1 <sup>i</sup> —Al7—Al10	64.4 (4)
Al10 <sup>i</sup> —Al1—Al13 <sup>ii</sup>	93.67 (4)	Al6—Al7—Al10	58.49 (2)
Al10 <sup>ii</sup> —Al1—Al13 <sup>ii</sup>	61.62 (3)	Al15 <sup>vii</sup> —Al7—Al10	156.82 (3)
Al5 <sup>iii</sup> —Al1—Al13 <sup>ii</sup>	92.77 (2)	Cr3 <sup>x</sup> —Al7—Al10	57.41 (2)
Al5 <sup>iv</sup> —Al1—Al13 <sup>ii</sup>	152.15 (3)	Al7 <sup>xii</sup> —Al7—Al10	91.572 (19)
Al2—Al1—Al13 <sup>ii</sup>	98.14 (4)	Al15 <sup>x</sup> —Al7—Al10	104.80 (3)
Al13 <sup>i</sup> —Al1—Al13 <sup>ii</sup>	59.58 (4)	Al8—Al7—Al10	105.13 (3)
C1—Al1—Cr1	168.4 (5)	Al16 <sup>xiii</sup> —Al7—Al10	56.13 (3)
Al3—Al1—Cr1	110.92 (4)	Al4 <sup>iv</sup> —Al7—Al10	116.56 (3)
Al10 <sup>i</sup> —Al1—Cr1	114.59 (3)	Cr2—Al7—Al10	103.63 (3)
Al10 <sup>ii</sup> —Al1—Cr1	114.59 (3)	Al5 <sup>viii</sup> —Al7—Al10	62.82 (2)
Al5 <sup>iii</sup> —Al1—Cr1	114.62 (3)	Al6—Al8—Al15 <sup>ix</sup>	105.08 (3)
Al5 <sup>iv</sup> —Al1—Cr1	114.62 (3)	Al6—Al8—Al15 <sup>x</sup>	105.08 (3)
Al2—Al1—Cr1	53.30 (3)	Al15 <sup>ix</sup> —Al8—Al15 <sup>x</sup>	120.04 (5)
Al13 <sup>i</sup> —Al1—Cr1	52.99 (2)	Al6—Al8—Cr3 <sup>ix</sup>	58.09 (3)
Al13 <sup>ii</sup> —Al1—Cr1	52.99 (2)	Al15 <sup>ix</sup> —Al8—Cr3 <sup>ix</sup>	54.50 (2)
Al2—Cr1—Al2 <sup>v</sup>	180.0	Al15 <sup>x</sup> —Al8—Cr3 <sup>ix</sup>	105.21 (3)
Al2—Cr1—Al13 <sup>i</sup>	113.76 (2)	Al6—Al8—Cr3 <sup>x</sup>	58.09 (3)
Al2 <sup>v</sup> —Cr1—Al13 <sup>i</sup>	66.24 (2)	Al15 <sup>ix</sup> —Al8—Cr3 <sup>x</sup>	105.21 (3)
Al2—Cr1—Al13 <sup>vi</sup>	66.24 (2)	Al15 <sup>x</sup> —Al8—Cr3 <sup>x</sup>	54.50 (2)
Al2 <sup>v</sup> —Cr1—Al13 <sup>vi</sup>	113.76 (2)	Cr3 <sup>ix</sup> —Al8—Cr3 <sup>x</sup>	58.24 (3)
Al13 <sup>i</sup> —Cr1—Al13 <sup>vi</sup>	180.0	Al6—Al8—Al15 <sup>vii</sup>	99.26 (4)
Al2—Cr1—Al13 <sup>vii</sup>	66.24 (2)	Al15 <sup>ix</sup> —Al8—Al15 <sup>vii</sup>	139.03 (4)
Al2 <sup>v</sup> —Cr1—Al13 <sup>vii</sup>	113.76 (2)	Al15 <sup>x</sup> —Al8—Al15 <sup>vii</sup>	83.48 (2)
Al13 <sup>i</sup> —Cr1—Al13 <sup>vii</sup>	112.57 (3)	Cr3 <sup>ix</sup> —Al8—Al15 <sup>vii</sup>	156.98 (4)
Al13 <sup>vi</sup> —Cr1—Al13 <sup>vii</sup>	67.43 (3)	Cr3 <sup>x</sup> —Al8—Al15 <sup>vii</sup>	115.62 (2)



Al2—Cr1—Al13 <sup>ii</sup>	113.76 (2)	Al6—Al8—Al15 <sup>vi</sup>	99.26 (4)
Al2 <sup>v</sup> —Cr1—Al13 <sup>ii</sup>	66.24 (2)	Al15 <sup>ix</sup> —Al8—Al15 <sup>vi</sup>	83.48 (2)
Al13 <sup>i</sup> —Cr1—Al13 <sup>ii</sup>	67.43 (3)	Al15 <sup>x</sup> —Al8—Al15 <sup>vi</sup>	139.03 (4)
Al13 <sup>vi</sup> —Cr1—Al13 <sup>ii</sup>	112.57 (3)	Cr3 <sup>ix</sup> —Al8—Al15 <sup>vi</sup>	115.62 (2)
Al13 <sup>vii</sup> —Cr1—Al13 <sup>ii</sup>	180.0	Cr3 <sup>x</sup> —Al8—Al15 <sup>vi</sup>	156.98 (4)
Al2—Cr1—Al12 <sup>vii</sup>	116.291 (16)	Al15 <sup>vii</sup> —Al8—Al15 <sup>vi</sup>	60.19 (4)
Al2 <sup>v</sup> —Cr1—Al12 <sup>vii</sup>	63.709 (16)	Al6—Al8—Al17 <sup>viii</sup>	59.39 (2)
Al13 <sup>i</sup> —Cr1—Al12 <sup>vii</sup>	62.79 (2)	Al15 <sup>ix</sup> —Al8—Al17 <sup>viii</sup>	60.91 (2)
Al13 <sup>vi</sup> —Cr1—Al12 <sup>vii</sup>	117.21 (2)	Al15 <sup>x</sup> —Al8—Al17 <sup>viii</sup>	161.70 (4)
Al13 <sup>vii</sup> —Cr1—Al12 <sup>vii</sup>	60.52 (2)	Cr3 <sup>ix</sup> —Al8—Al17 <sup>viii</sup>	59.28 (2)
Al13 <sup>ii</sup> —Cr1—Al12 <sup>vii</sup>	119.48 (2)	Cr3 <sup>x</sup> —Al8—Al17 <sup>viii</sup>	107.20 (3)
Al2—Cr1—Al12 <sup>ii</sup>	63.709 (16)	Al15 <sup>vii</sup> —Al8—Al17 <sup>viii</sup>	107.45 (4)
Al2 <sup>v</sup> —Cr1—Al12 <sup>ii</sup>	116.292 (16)	Al15 <sup>vi</sup> —Al8—Al17 <sup>viii</sup>	57.92 (2)
Al13 <sup>i</sup> —Cr1—Al12 <sup>ii</sup>	117.21 (2)	Al6—Al8—Al17	59.39 (2)
Al13 <sup>vi</sup> —Cr1—Al12 <sup>ii</sup>	62.79 (2)	Al15 <sup>ix</sup> —Al8—Al17	161.70 (4)
Al13 <sup>vii</sup> —Cr1—Al12 <sup>ii</sup>	119.48 (2)	Al15 <sup>x</sup> —Al8—Al17	60.91 (2)
Al13 <sup>ii</sup> —Cr1—Al12 <sup>ii</sup>	60.52 (2)	Cr3 <sup>ix</sup> —Al8—Al17	107.20 (3)
Al12 <sup>vii</sup> —Cr1—Al12 <sup>ii</sup>	180.0	Cr3 <sup>x</sup> —Al8—Al17	59.28 (2)
Al2—Cr1—Al12 <sup>vi</sup>	116.291 (16)	Al15 <sup>vii</sup> —Al8—Al17	57.92 (2)
Al2 <sup>v</sup> —Cr1—Al12 <sup>vi</sup>	63.709 (16)	Al15 <sup>vi</sup> —Al8—Al17	107.45 (4)
Al13 <sup>i</sup> —Cr1—Al12 <sup>vi</sup>	119.48 (2)	Al17 <sup>viii</sup> —Al8—Al17	111.93 (4)
Al13 <sup>vi</sup> —Cr1—Al12 <sup>vi</sup>	60.52 (2)	Al6—Al8—Al14 <sup>ix</sup>	104.00 (4)
Al13 <sup>vii</sup> —Cr1—Al12 <sup>vi</sup>	117.21 (2)	Al15 <sup>ix</sup> —Al8—Al14 <sup>ix</sup>	61.52 (2)
Al13 <sup>ii</sup> —Cr1—Al12 <sup>vi</sup>	62.79 (2)	Al15 <sup>x</sup> —Al8—Al14 <sup>ix</sup>	61.52 (2)
Al12 <sup>vii</sup> —Cr1—Al12 <sup>vi</sup>	117.56 (3)	Cr3 <sup>ix</sup> —Al8—Al14 <sup>ix</sup>	56.83 (2)
Al12 <sup>ii</sup> —Cr1—Al12 <sup>vi</sup>	62.44 (3)	Cr3 <sup>x</sup> —Al8—Al14 <sup>ix</sup>	56.83 (2)
Al2—Cr1—Al12 <sup>i</sup>	63.709 (16)	Al15 <sup>vii</sup> —Al8—Al14 <sup>ix</sup>	141.81 (3)
Al2 <sup>v</sup> —Cr1—Al12 <sup>i</sup>	116.291 (16)	Al15 <sup>vi</sup> —Al8—Al14 <sup>ix</sup>	141.81 (3)
Al13 <sup>i</sup> —Cr1—Al12 <sup>i</sup>	60.52 (2)	Al17 <sup>viii</sup> —Al8—Al14 <sup>ix</sup>	110.40 (3)
Al13 <sup>vi</sup> —Cr1—Al12 <sup>i</sup>	119.48 (2)	Al7—Al8—Al14 <sup>ix</sup>	110.40 (3)
Al13 <sup>vii</sup> —Cr1—Al12 <sup>i</sup>	62.79 (2)	Al6—Al8—Cr2	53.73 (3)
Al13 <sup>ii</sup> —Cr1—Al12 <sup>i</sup>	117.21 (2)	Al15 <sup>ix</sup> —Al8—Cr2	119.86 (2)
Al12 <sup>vii</sup> —Cr1—Al12 <sup>i</sup>	62.44 (3)	Al15 <sup>x</sup> —Al8—Cr2	119.86 (2)
Al12 <sup>ii</sup> —Cr1—Al12 <sup>i</sup>	117.56 (3)	Cr3 <sup>ix</sup> —Al8—Cr2	104.37 (3)
Al12 <sup>vi</sup> —Cr1—Al12 <sup>i</sup>	180.0	Cr3 <sup>x</sup> —Al8—Cr2	104.37 (3)
Al2—Cr1—Al1 <sup>v</sup>	118.14 (3)	Al15 <sup>vii</sup> —Al8—Cr2	53.82 (2)
Al2 <sup>v</sup> —Cr1—Al1 <sup>v</sup>	61.86 (3)	Al15 <sup>vi</sup> —Al8—Cr2	53.82 (2)
Al13 <sup>i</sup> —Cr1—Al1 <sup>v</sup>	116.85 (2)	Al17 <sup>viii</sup> —Al8—Cr2	60.75 (2)
Al13 <sup>vi</sup> —Cr1—Al1 <sup>v</sup>	63.15 (2)	Al7—Al8—Cr2	60.75 (2)
Al13 <sup>vii</sup> —Cr1—Al1 <sup>v</sup>	63.15 (2)	Al14 <sup>ix</sup> —Al8—Cr2	157.73 (4)
Al13 <sup>ii</sup> —Cr1—Al1 <sup>v</sup>	116.85 (2)	Al6—Al9—Al6 <sup>ix</sup>	180.00 (4)
Al12 <sup>vii</sup> —Cr1—Al1 <sup>v</sup>	63.491 (16)	Al6—Al9—Cr3	118.398 (19)
Al12 <sup>ii</sup> —Cr1—Al1 <sup>v</sup>	116.509 (16)	Al6 <sup>ix</sup> —Al9—Cr3	61.602 (19)
Al12 <sup>vi</sup> —Cr1—Al1 <sup>v</sup>	63.491 (16)	Al6—Al9—Cr3 <sup>viii</sup>	118.399 (19)
Al12 <sup>i</sup> —Cr1—Al1 <sup>v</sup>	116.509 (16)	Al6 <sup>ix</sup> —Al9—Cr3 <sup>viii</sup>	61.601 (19)
Al2—Cr1—Al1	61.86 (3)	Cr3—Al9—Cr3 <sup>viii</sup>	62.622 (17)
Al2 <sup>v</sup> —Cr1—Al1	118.14 (3)	Al6—Al9—Cr3 <sup>x</sup>	61.601 (19)
Al13 <sup>i</sup> —Cr1—Al1	63.15 (2)	Al6 <sup>ix</sup> —Al9—Cr3 <sup>x</sup>	118.399 (19)

Al13 <sup>vi</sup> —Cr1—Al1	116.85 (2)	Cr3—Al9—Cr3 <sup>x</sup>	117.378 (17)
Al13 <sup>vii</sup> —Cr1—Al1	116.85 (2)	Cr3 <sup>viii</sup> —Al9—Cr3 <sup>x</sup>	180.0
Al13 <sup>ii</sup> —Cr1—Al1	63.15 (2)	Al6—Al9—Cr3 <sup>ix</sup>	61.601 (19)
Al12 <sup>vii</sup> —Cr1—Al1	116.509 (16)	Al6 <sup>ix</sup> —Al9—Cr3 <sup>ix</sup>	118.399 (19)
Al12 <sup>ii</sup> —Cr1—Al1	63.491 (16)	Cr3—Al9—Cr3 <sup>ix</sup>	180.0
Al12 <sup>vi</sup> —Cr1—Al1	116.509 (16)	Cr3 <sup>viii</sup> —Al9—Cr3 <sup>ix</sup>	117.378 (17)
Al12 <sup>i</sup> —Cr1—Al1	63.491 (16)	Cr3 <sup>x</sup> —Al9—Cr3 <sup>ix</sup>	62.622 (17)
Al1 <sup>v</sup> —Cr1—Al1	180.0	Al6—Al9—Al10	64.439 (17)
Al1—C1—Al3	80.1 (6)	Al6 <sup>ix</sup> —Al9—Al10	115.561 (16)
Al1—C1—Al7 <sup>i</sup>	132.0 (6)	Cr3—Al9—Al10	63.724 (17)
Al3—C1—Al7 <sup>i</sup>	123.7 (6)	Cr3 <sup>viii</sup> —Al9—Al10	116.514 (17)
Al1—C1—Al7 <sup>ii</sup>	132.0 (6)	Cr3 <sup>x</sup> —Al9—Al10	63.486 (17)
Al3—C1—Al7 <sup>ii</sup>	123.7 (6)	Cr3 <sup>ix</sup> —Al9—Al10	116.276 (18)
Al7 <sup>i</sup> —C1—Al7 <sup>ii</sup>	72.8 (5)	Al6—Al9—Al10 <sup>ix</sup>	115.562 (16)
Al1—C1—Al5 <sup>iii</sup>	77.1 (4)	Al6 <sup>ix</sup> —Al9—Al10 <sup>ix</sup>	64.438 (17)
Al3—C1—Al5 <sup>iii</sup>	71.6 (4)	Cr3—Al9—Al10 <sup>ix</sup>	116.274 (18)
Al7 <sup>i</sup> —C1—Al5 <sup>iii</sup>	146.0 (6)	Cr3 <sup>viii</sup> —Al9—Al10 <sup>ix</sup>	63.485 (17)
Al7 <sup>ii</sup> —C1—Al5 <sup>iii</sup>	73.79 (13)	Cr3 <sup>x</sup> —Al9—Al10 <sup>ix</sup>	116.515 (17)
Al1—C1—Al5 <sup>iv</sup>	77.1 (4)	Cr3 <sup>ix</sup> —Al9—Al10 <sup>ix</sup>	63.726 (17)
Al3—C1—Al5 <sup>iv</sup>	71.6 (4)	Al10—Al9—Al10 <sup>ix</sup>	180.0
Al7 <sup>i</sup> —C1—Al5 <sup>iv</sup>	73.79 (13)	Al6—Al9—Al10 <sup>viii</sup>	64.438 (16)
Al7 <sup>ii</sup> —C1—Al5 <sup>iv</sup>	146.0 (6)	Al6 <sup>ix</sup> —Al9—Al10 <sup>viii</sup>	115.562 (17)
Al5 <sup>iii</sup> —C1—Al5 <sup>iv</sup>	137.9 (7)	Cr3—Al9—Al10 <sup>viii</sup>	116.515 (17)
Cr2—Al2—Cr1	174.84 (4)	Cr3 <sup>viii</sup> —Al9—Al10 <sup>viii</sup>	63.726 (17)
Cr2—Al2—Al3	60.58 (3)	Cr3 <sup>x</sup> —Al9—Al10 <sup>viii</sup>	116.274 (17)
Cr1—Al2—Al3	124.58 (4)	Cr3 <sup>ix</sup> —Al9—Al10 <sup>viii</sup>	63.485 (17)
Cr2—Al2—Al13 <sup>vii</sup>	118.78 (4)	Al10—Al9—Al10 <sup>viii</sup>	117.61 (3)
Cr1—Al2—Al13 <sup>vii</sup>	57.07 (2)	Al10 <sup>ix</sup> —Al9—Al10 <sup>viii</sup>	62.39 (3)
Al3—Al2—Al13 <sup>vii</sup>	149.091 (19)	Al6—Al9—Al10 <sup>x</sup>	115.562 (17)
Cr2—Al2—Al13 <sup>vi</sup>	118.78 (4)	Al6 <sup>ix</sup> —Al9—Al10 <sup>x</sup>	64.438 (16)
Cr1—Al2—Al13 <sup>vi</sup>	57.07 (2)	Cr3—Al9—Al10 <sup>x</sup>	63.485 (17)
Al3—Al2—Al13 <sup>vi</sup>	149.091 (19)	Cr3 <sup>viii</sup> —Al9—Al10 <sup>x</sup>	116.274 (17)
Al13 <sup>vii</sup> —Al2—Al13 <sup>vi</sup>	61.20 (3)	Cr3 <sup>x</sup> —Al9—Al10 <sup>x</sup>	63.726 (17)
Cr2—Al2—Al1	120.32 (4)	Cr3 <sup>ix</sup> —Al9—Al10 <sup>x</sup>	116.515 (17)
Cr1—Al2—Al1	64.84 (3)	Al10—Al9—Al10 <sup>x</sup>	62.39 (3)
Al3—Al2—Al1	59.74 (4)	Al10 <sup>ix</sup> —Al9—Al10 <sup>x</sup>	117.61 (3)
Al13 <sup>vii</sup> —Al2—Al1	111.89 (4)	Al10 <sup>viii</sup> —Al9—Al10 <sup>x</sup>	180.0
Al13 <sup>vi</sup> —Al2—Al1	111.89 (4)	Al6—Al9—Al11 <sup>ix</sup>	115.09 (3)
Cr2—Al2—Al4 <sup>iii</sup>	59.96 (2)	Al6 <sup>ix</sup> —Al9—Al11 <sup>ix</sup>	64.91 (3)
Cr1—Al2—Al4 <sup>iii</sup>	121.22 (2)	Cr3—Al9—Al11 <sup>ix</sup>	116.175 (18)
Al3—Al2—Al4 <sup>iii</sup>	64.10 (2)	Cr3 <sup>viii</sup> —Al9—Al11 <sup>ix</sup>	116.174 (18)
Al13 <sup>vii</sup> —Al2—Al4 <sup>iii</sup>	145.46 (4)	Cr3 <sup>x</sup> —Al9—Al11 <sup>ix</sup>	63.825 (18)
Al13 <sup>vi</sup> —Al2—Al4 <sup>iii</sup>	88.34 (2)	Cr3 <sup>ix</sup> —Al9—Al11 <sup>ix</sup>	63.825 (18)
Al1—Al2—Al4 <sup>iii</sup>	93.64 (3)	Al10—Al9—Al11 <sup>ix</sup>	116.259 (16)
Cr2—Al2—Al4 <sup>iv</sup>	59.96 (2)	Al10 <sup>ix</sup> —Al9—Al11 <sup>ix</sup>	63.742 (16)
Cr1—Al2—Al4 <sup>iv</sup>	121.22 (2)	Al10 <sup>viii</sup> —Al9—Al11 <sup>ix</sup>	116.258 (16)
Al3—Al2—Al4 <sup>iv</sup>	64.10 (2)	Al10 <sup>x</sup> —Al9—Al11 <sup>ix</sup>	63.742 (16)
Al13 <sup>vii</sup> —Al2—Al4 <sup>iv</sup>	88.34 (2)	Al6—Al9—Al11	64.91 (3)

Al13 <sup>vi</sup> —Al2—Al4 <sup>iv</sup>	145.46 (4)	Al6 <sup>ix</sup> —Al9—Al11	115.09 (3)
Al1—Al2—Al4 <sup>iv</sup>	93.64 (3)	Cr3—Al9—Al11	63.824 (18)
Al4 <sup>iii</sup> —Al2—Al4 <sup>iv</sup>	113.74 (4)	Cr3 <sup>viii</sup> —Al9—Al11	63.824 (18)
Cr2—Al2—Al12 <sup>i</sup>	118.85 (2)	Cr3 <sup>x</sup> —Al9—Al11	116.176 (19)
Cr1—Al2—Al12 <sup>i</sup>	62.58 (2)	Cr3 <sup>ix</sup> —Al9—Al11	116.176 (18)
Al3—Al2—Al12 <sup>i</sup>	92.40 (3)	Al10—Al9—Al11	63.742 (16)
Al13 <sup>vii</sup> —Al2—Al12 <sup>i</sup>	59.77 (2)	Al10 <sup>ix</sup> —Al9—Al11	116.258 (16)
Al13 <sup>vi</sup> —Al2—Al12 <sup>i</sup>	111.01 (4)	Al10 <sup>viii</sup> —Al9—Al11	63.742 (16)
Al1—Al2—Al12 <sup>i</sup>	64.08 (2)	Al10 <sup>x</sup> —Al9—Al11	116.258 (16)
Al4 <sup>iii</sup> —Al2—Al12 <sup>i</sup>	154.36 (4)	Al11 <sup>ix</sup> —Al9—Al11	180.0
Al4 <sup>iv</sup> —Al2—Al12 <sup>i</sup>	58.90 (2)	Al9—Al10—Al1 <sup>i</sup>	151.34 (3)
Cr2—Al2—Al12 <sup>ii</sup>	118.85 (2)	Al9—Al10—Al16 <sup>xiii</sup>	103.24 (3)
Cr1—Al2—Al12 <sup>ii</sup>	62.58 (2)	Al1 <sup>i</sup> —Al10—Al16 <sup>xiii</sup>	104.64 (3)
Al3—Al2—Al12 <sup>ii</sup>	92.40 (3)	Al9—Al10—Cr3 <sup>x</sup>	56.225 (16)
Al13 <sup>vii</sup> —Al2—Al12 <sup>ii</sup>	111.01 (4)	Al1 <sup>i</sup> —Al10—Cr3 <sup>x</sup>	142.69 (3)
Al13 <sup>vi</sup> —Al2—Al12 <sup>ii</sup>	59.77 (2)	Al16 <sup>xiii</sup> —Al10—Cr3 <sup>x</sup>	53.119 (19)
Al1—Al2—Al12 <sup>ii</sup>	64.08 (2)	Al9—Al10—Cr3	56.114 (16)
Al4 <sup>iii</sup> —Al2—Al12 <sup>ii</sup>	58.90 (2)	Al1 <sup>i</sup> —Al10—Cr3	112.51 (3)
Al4 <sup>iv</sup> —Al2—Al12 <sup>ii</sup>	154.36 (4)	Al16 <sup>xiii</sup> —Al10—Cr3	121.35 (3)
Al12 <sup>i</sup> —Al2—Al12 <sup>ii</sup>	115.71 (4)	Cr3 <sup>x</sup> —Al10—Cr3	104.80 (3)
Cr2—Al2—Al15 <sup>vi</sup>	56.50 (2)	Al9—Al10—Al10 <sup>x</sup>	58.807 (15)
Cr1—Al2—Al15 <sup>vi</sup>	119.25 (3)	Al1 <sup>i</sup> —Al10—Al10 <sup>x</sup>	142.92 (3)
Al3—Al2—Al15 <sup>vi</sup>	108.67 (4)	Al16 <sup>xiii</sup> —Al10—Al10 <sup>x</sup>	63.13 (3)
Al13 <sup>vii</sup> —Al2—Al15 <sup>vi</sup>	91.60 (3)	Cr3 <sup>x</sup> —Al10—Al10 <sup>x</sup>	60.04 (2)
Al13 <sup>vi</sup> —Al2—Al15 <sup>vi</sup>	62.28 (3)	Cr3—Al10—Al10 <sup>x</sup>	59.71 (2)
Al1—Al2—Al15 <sup>vi</sup>	149.83 (2)	Al9—Al10—Al6	55.71 (2)
Al4 <sup>iii</sup> —Al2—Al15 <sup>vi</sup>	57.78 (2)	Al1 <sup>i</sup> —Al10—Al6	111.43 (3)
Al4 <sup>iv</sup> —Al2—Al15 <sup>vi</sup>	106.15 (4)	Al16 <sup>xiii</sup> —Al10—Al6	101.84 (3)
Al12 <sup>i</sup> —Al2—Al15 <sup>vi</sup>	145.96 (3)	Cr3 <sup>x</sup> —Al10—Al6	56.36 (2)
Al12 <sup>ii</sup> —Al2—Al15 <sup>vi</sup>	90.47 (2)	Cr3—Al10—Al6	104.55 (3)
Cr2—Al2—Al15 <sup>vii</sup>	56.50 (2)	Al10 <sup>x</sup> —Al10—Al6	105.46 (3)
Cr1—Al2—Al15 <sup>vii</sup>	119.25 (3)	Al9—Al10—Al11	58.45 (2)
Al3—Al2—Al15 <sup>vii</sup>	108.67 (4)	Al1 <sup>i</sup> —Al10—Al11	92.92 (3)
Al13 <sup>vii</sup> —Al2—Al15 <sup>vii</sup>	62.28 (3)	Al16 <sup>xiii</sup> —Al10—Al11	158.95 (3)
Al13 <sup>vi</sup> —Al2—Al15 <sup>vii</sup>	91.60 (3)	Cr3 <sup>x</sup> —Al10—Al11	105.83 (3)
Al1—Al2—Al15 <sup>vii</sup>	149.83 (2)	Cr3—Al10—Al11	59.50 (2)
Al4 <sup>iii</sup> —Al2—Al15 <sup>vii</sup>	106.15 (4)	Al10 <sup>x</sup> —Al10—Al11	108.84 (3)
Al4 <sup>iv</sup> —Al2—Al15 <sup>vii</sup>	57.78 (2)	Al6—Al10—Al11	60.15 (3)
Al12 <sup>i</sup> —Al2—Al15 <sup>vii</sup>	90.47 (2)	Al9—Al10—Al13	99.06 (3)
Al12 <sup>ii</sup> —Al2—Al15 <sup>vii</sup>	145.96 (3)	Al1 <sup>i</sup> —Al10—Al13	61.40 (3)
Al15 <sup>vi</sup> —Al2—Al15 <sup>vii</sup>	57.95 (3)	Al16 <sup>xiii</sup> —Al10—Al13	142.42 (3)
Al2—Cr2—Al6	179.44 (4)	Cr3 <sup>x</sup> —Al10—Al13	154.94 (3)
Al2—Cr2—Al15 <sup>vii</sup>	70.31 (3)	Cr3—Al10—Al13	51.77 (2)
Al6—Cr2—Al15 <sup>vii</sup>	110.14 (3)	Al10 <sup>x</sup> —Al10—Al13	105.58 (4)
Al2—Cr2—Al15 <sup>vi</sup>	70.31 (3)	Al6—Al10—Al13	115.72 (3)
Al6—Cr2—Al15 <sup>vi</sup>	110.14 (3)	Al11—Al10—Al13	56.97 (2)
Al15 <sup>vii</sup> —Cr2—Al15 <sup>vi</sup>	66.32 (3)	Al9—Al10—Al16	99.50 (3)
Al2—Cr2—Al3	63.54 (3)	Al1 <sup>i</sup> —Al10—Al16	88.14 (3)

Al6—Cr2—Al3	115.90 (3)	Al16 <sup>xiii</sup> —Al10—Al16	87.65 (3)
Al15 <sup>vii</sup> —Cr2—Al3	122.41 (3)	Cr3 <sup>x</sup> —Al10—Al16	116.63 (3)
Al15 <sup>vi</sup> —Cr2—Al3	122.41 (3)	Cr3—Al10—Al16	51.518 (19)
Al2—Cr2—Al4 <sup>iv</sup>	66.693 (19)	Al10 <sup>x</sup> —Al10—Al16	57.94 (3)
Al6—Cr2—Al4 <sup>iv</sup>	113.164 (19)	Al6—Al10—Al16	154.76 (3)
Al15 <sup>vii</sup> —Cr2—Al4 <sup>iv</sup>	63.83 (2)	Al11—Al10—Al16	104.71 (3)
Al15 <sup>vi</sup> —Cr2—Al4 <sup>iv</sup>	122.06 (3)	Al13—Al10—Al16	58.86 (3)
Al3—Cr2—Al4 <sup>iv</sup>	67.392 (19)	Al9—Al10—Al17	102.79 (3)
Al2—Cr2—Al4 <sup>iii</sup>	66.693 (19)	Al1 <sup>i</sup> —Al10—Al17	85.56 (3)
Al6—Cr2—Al4 <sup>iii</sup>	113.164 (19)	Al16 <sup>xiii</sup> —Al10—Al17	60.20 (3)
Al15 <sup>vii</sup> —Cr2—Al4 <sup>iii</sup>	122.06 (3)	Cr3 <sup>x</sup> —Al10—Al17	57.82 (2)
Al15 <sup>vi</sup> —Cr2—Al4 <sup>iii</sup>	63.83 (2)	Cr3—Al10—Al17	158.89 (3)
Al3—Cr2—Al4 <sup>iii</sup>	67.392 (19)	Al10 <sup>x</sup> —Al10—Al17	112.47 (4)
Al4 <sup>iv</sup> —Cr2—Al4 <sup>iii</sup>	125.37 (4)	Al6—Al10—Al17	56.81 (2)
Al2—Cr2—Al5	116.68 (3)	Al11—Al10—Al17	110.80 (3)
Al6—Cr2—Al5	62.87 (3)	Al13—Al10—Al17	141.83 (3)
Al15 <sup>vii</sup> —Cr2—Al5	172.81 (3)	Al16—Al10—Al17	144.18 (3)
Al15 <sup>vi</sup> —Cr2—Al5	113.55 (2)	Al9—Al10—Al10 <sup>xii</sup>	148.807 (15)
Al3—Cr2—Al5	64.15 (2)	Al1 <sup>i</sup> —Al10—Al10 <sup>xii</sup>	57.129 (19)
Al4 <sup>iv</sup> —Cr2—Al5	119.58 (3)	Al16 <sup>xiii</sup> —Al10—Al10 <sup>xii</sup>	57.218 (19)
Al4 <sup>iii</sup> —Cr2—Al5	62.05 (2)	Cr3 <sup>x</sup> —Al10—Al10 <sup>xii</sup>	110.336 (17)
Al2—Cr2—Al5 <sup>viii</sup>	116.68 (3)	Cr3—Al10—Al10 <sup>xii</sup>	110.268 (17)
Al6—Cr2—Al5 <sup>viii</sup>	62.87 (2)	Al10 <sup>x</sup> —Al10—Al10 <sup>xii</sup>	90.0
Al15 <sup>vii</sup> —Cr2—Al5 <sup>viii</sup>	113.55 (2)	Al6—Al10—Al10 <sup>xii</sup>	145.07 (2)
Al15 <sup>vi</sup> —Cr2—Al5 <sup>viii</sup>	172.81 (3)	Al11—Al10—Al10 <sup>xii</sup>	143.83 (2)
Al3—Cr2—Al5 <sup>viii</sup>	64.15 (2)	Al13—Al10—Al10 <sup>xii</sup>	88.77 (2)
Al4 <sup>iv</sup> —Cr2—Al5 <sup>viii</sup>	62.05 (2)	Al16—Al10—Al10 <sup>xii</sup>	59.044 (17)
Al4 <sup>iii</sup> —Cr2—Al5 <sup>viii</sup>	119.58 (3)	Al7—Al10—Al10 <sup>xii</sup>	88.427 (19)
Al5—Cr2—Al5 <sup>viii</sup>	65.59 (3)	Al9—Al11—Al13	102.43 (3)
Al2—Cr2—Al8	121.79 (3)	Al9—Al11—Al13 <sup>viii</sup>	102.43 (3)
Al6—Cr2—Al8	58.77 (3)	Al13—Al11—Al13 <sup>viii</sup>	119.49 (4)
Al15 <sup>vii</sup> —Cr2—Al8	61.71 (2)	Al9—Al11—Cr3	55.75 (2)
Al15 <sup>vi</sup> —Cr2—Al8	61.71 (2)	Al13—Al11—Cr3	53.17 (2)
Al3—Cr2—Al8	174.67 (3)	Al13 <sup>viii</sup> —Al11—Cr3	103.15 (3)
Al4 <sup>iv</sup> —Cr2—Al8	113.958 (19)	Al9—Al11—Cr3 <sup>viii</sup>	55.75 (2)
Al4 <sup>iii</sup> —Cr2—Al8	113.958 (19)	Al13—Al11—Cr3 <sup>viii</sup>	103.15 (3)
Al5—Cr2—Al8	111.55 (3)	Al13 <sup>viii</sup> —Al11—Cr3 <sup>viii</sup>	53.17 (2)
Al5 <sup>viii</sup> —Cr2—Al8	111.55 (3)	Cr3—Al11—Cr3 <sup>viii</sup>	57.20 (2)
Al2—Cr2—Al7 <sup>viii</sup>	119.827 (19)	Al9—Al11—Al12	148.15 (2)
Al6—Cr2—Al7 <sup>viii</sup>	60.363 (18)	Al13—Al11—Al12	58.97 (2)
Al15 <sup>vii</sup> —Cr2—Al7 <sup>viii</sup>	113.04 (3)	Al13 <sup>viii</sup> —Al11—Al12	109.26 (4)
Al15 <sup>vi</sup> —Cr2—Al7 <sup>viii</sup>	59.83 (2)	Cr3—Al11—Al12	112.14 (2)
Al3—Cr2—Al7 <sup>viii</sup>	118.832 (19)	Cr3 <sup>viii</sup> —Al11—Al12	147.70 (4)
Al4 <sup>iv</sup> —Cr2—Al7 <sup>viii</sup>	172.12 (3)	Al9—Al11—Al12 <sup>viii</sup>	148.15 (2)
Al4 <sup>iii</sup> —Cr2—Al7 <sup>viii</sup>	62.51 (2)	Al13—Al11—Al12 <sup>viii</sup>	109.26 (4)
Al5—Cr2—Al7 <sup>viii</sup>	62.67 (2)	Al13 <sup>viii</sup> —Al11—Al12 <sup>viii</sup>	58.97 (2)
Al5 <sup>viii</sup> —Cr2—Al7 <sup>viii</sup>	115.22 (3)	Cr3—Al11—Al12 <sup>viii</sup>	147.70 (4)
Al8—Cr2—Al7 <sup>viii</sup>	59.370 (18)	Cr3 <sup>viii</sup> —Al11—Al12 <sup>viii</sup>	112.14 (2)

Al2—Cr2—Al7	119.827 (19)	Al12—Al11—Al12 <sup>viii</sup>	58.60 (4)
Al6—Cr2—Al7	60.363 (18)	Al9—Al11—Al6	55.19 (3)
Al15 <sup>vii</sup> —Cr2—Al7	59.83 (2)	Al13—Al11—Al6	119.79 (2)
Al15 <sup>vi</sup> —Cr2—Al7	113.04 (3)	Al13 <sup>viii</sup> —Al11—Al6	119.80 (2)
Al3—Cr2—Al7	118.831 (19)	Cr3—Al11—Al6	103.42 (3)
Al4 <sup>iv</sup> —Cr2—Al7	62.51 (2)	Cr3 <sup>viii</sup> —Al11—Al6	103.42 (3)
Al4 <sup>iii</sup> —Cr2—Al7	172.13 (3)	Al12—Al11—Al6	108.84 (4)
Al5—Cr2—Al7	115.22 (3)	Al12 <sup>viii</sup> —Al11—Al6	108.84 (4)
Al5 <sup>viii</sup> —Cr2—Al7	62.67 (2)	Al9—Al11—Al10	57.81 (2)
Al8—Cr2—Al7	59.371 (18)	Al13—Al11—Al10	62.17 (2)
Al7 <sup>viii</sup> —Cr2—Al7	109.62 (3)	Al13 <sup>viii</sup> —Al11—Al10	158.08 (4)
C1—Al3—Cr2	160.9 (4)	Cr3—Al11—Al10	59.01 (2)
C1—Al3—Al4	71.5 (3)	Cr3 <sup>viii</sup> —Al11—Al10	104.95 (3)
Cr2—Al3—Al4	123.89 (4)	Al12—Al11—Al10	90.42 (2)
C1—Al3—Al4 <sup>viii</sup>	71.5 (3)	Al12 <sup>viii</sup> —Al11—Al10	142.88 (4)
Cr2—Al3—Al4 <sup>viii</sup>	123.89 (4)	Al6—Al11—Al10	59.15 (2)
Al4—Al3—Al4 <sup>viii</sup>	64.16 (4)	Al9—Al11—Al10 <sup>viii</sup>	57.81 (2)
C1—Al3—Al2	105.0 (4)	Al13—Al11—Al10 <sup>viii</sup>	158.08 (4)
Cr2—Al3—Al2	55.88 (3)	Al13 <sup>viii</sup> —Al11—Al10 <sup>viii</sup>	62.17 (2)
Al4—Al3—Al2	147.24 (2)	Cr3—Al11—Al10 <sup>viii</sup>	104.95 (3)
Al4 <sup>viii</sup> —Al3—Al2	147.24 (2)	Cr3 <sup>viii</sup> —Al11—Al10 <sup>viii</sup>	59.01 (2)
C1—Al3—Al1	42.4 (4)	Al12—Al11—Al10 <sup>viii</sup>	142.88 (4)
Cr2—Al3—Al1	118.52 (4)	Al12 <sup>viii</sup> —Al11—Al10 <sup>viii</sup>	90.42 (2)
Al4—Al3—Al1	107.12 (4)	Al6—Al11—Al10 <sup>viii</sup>	59.15 (2)
Al4 <sup>viii</sup> —Al3—Al1	107.12 (4)	Al10—Al11—Al10 <sup>viii</sup>	107.66 (4)
Al2—Al3—Al1	62.64 (4)	Al9—Al11—Al14	101.16 (4)
C1—Al3—Al5	134.8 (3)	Al13—Al11—Al14	60.75 (2)
Cr2—Al3—Al5	59.50 (3)	Al13 <sup>viii</sup> —Al11—Al14	60.75 (2)
Al4—Al3—Al5	64.44 (3)	Cr3—Al11—Al14	56.48 (3)
Al4 <sup>viii</sup> —Al3—Al5	96.86 (4)	Cr3 <sup>viii</sup> —Al11—Al14	56.48 (3)
Al2—Al3—Al5	106.56 (4)	Al12—Al11—Al14	91.67 (3)
Al1—Al3—Al5	147.88 (2)	Al12 <sup>viii</sup> —Al11—Al14	91.67 (3)
C1—Al3—Al5 <sup>viii</sup>	134.8 (3)	Al6—Al11—Al14	156.35 (5)
Cr2—Al3—Al5 <sup>viii</sup>	59.50 (3)	Al10—Al11—Al14	110.64 (3)
Al4—Al3—Al5 <sup>viii</sup>	96.86 (4)	Al10 <sup>viii</sup> —Al11—Al14	110.64 (3)
Al4 <sup>viii</sup> —Al3—Al5 <sup>viii</sup>	64.44 (3)	Al13—Al12—Al12 <sup>viii</sup>	111.17 (2)
Al2—Al3—Al5 <sup>viii</sup>	106.56 (4)	Al13—Al12—Al5 <sup>viii</sup>	95.39 (3)
Al1—Al3—Al5 <sup>viii</sup>	147.88 (2)	Al12 <sup>viii</sup> —Al12—Al5 <sup>viii</sup>	91.79 (2)
Al5—Al3—Al5 <sup>viii</sup>	62.48 (4)	Al13—Al12—Al4 <sup>viii</sup>	150.32 (4)
C1—Al3—Al5 <sup>iv</sup>	56.60 (8)	Al12 <sup>viii</sup> —Al12—Al4 <sup>viii</sup>	90.78 (2)
Cr2—Al3—Al5 <sup>iv</sup>	118.09 (2)	Al5 <sup>viii</sup> —Al12—Al4 <sup>viii</sup>	63.06 (3)
Al4—Al3—Al5 <sup>iv</sup>	112.29 (4)	Al13—Al12—Al11	59.11 (2)
Al4 <sup>viii</sup> —Al3—Al5 <sup>iv</sup>	60.46 (2)	Al12 <sup>viii</sup> —Al12—Al11	60.703 (18)
Al2—Al3—Al5 <sup>iv</sup>	89.84 (3)	Al5 <sup>viii</sup> —Al12—Al11	68.95 (3)
Al1—Al3—Al5 <sup>iv</sup>	59.46 (2)	Al4 <sup>viii</sup> —Al12—Al11	122.62 (3)
Al5—Al3—Al5 <sup>iv</sup>	152.46 (3)	Al13—Al12—Al13 <sup>xiv</sup>	101.04 (3)
Al5 <sup>viii</sup> —Al3—Al5 <sup>iv</sup>	92.00 (2)	Al12 <sup>viii</sup> —Al12—Al13 <sup>xiv</sup>	110.45 (2)
C1—Al3—Al5 <sup>iii</sup>	56.60 (8)	Al5 <sup>viii</sup> —Al12—Al13 <sup>xiv</sup>	144.83 (3)

Cr2—Al3—Al5 <sup>iii</sup>	118.09 (2)	Al4 <sup>viii</sup> —Al12—Al13 <sup>xiv</sup>	88.90 (3)
Al4—Al3—Al5 <sup>iii</sup>	60.46 (2)	Al11—Al12—Al13 <sup>xiv</sup>	145.66 (4)
Al4 <sup>viii</sup> —Al3—Al5 <sup>iii</sup>	112.29 (4)	Al13—Al12—Cr1 <sup>xv</sup>	55.22 (2)
Al2—Al3—Al5 <sup>iii</sup>	89.84 (3)	Al12 <sup>viii</sup> —Al12—Cr1 <sup>xv</sup>	148.779 (15)
Al1—Al3—Al5 <sup>iii</sup>	59.46 (2)	Al5 <sup>viii</sup> —Al12—Cr1 <sup>xv</sup>	115.97 (3)
Al5—Al3—Al5 <sup>iii</sup>	92.00 (2)	Al4 <sup>viii</sup> —Al12—Cr1 <sup>xv</sup>	113.79 (3)
Al5 <sup>viii</sup> —Al3—Al5 <sup>iii</sup>	152.46 (3)	Al11—Al12—Cr1 <sup>xv</sup>	114.33 (3)
Al5 <sup>iv</sup> —Al3—Al5 <sup>iii</sup>	110.41 (4)	Al13 <sup>xiv</sup> —Al12—Cr1 <sup>xv</sup>	54.284 (19)
C1—Al3—Al4 <sup>iii</sup>	115.75 (18)	Al13—Al12—Al2 <sup>i</sup>	100.90 (3)
Cr2—Al3—Al4 <sup>iii</sup>	57.38 (2)	Al12 <sup>viii</sup> —Al12—Al2 <sup>i</sup>	147.85 (2)
Al4—Al3—Al4 <sup>iii</sup>	90.91 (2)	Al5 <sup>viii</sup> —Al12—Al2 <sup>i</sup>	87.22 (3)
Al4 <sup>viii</sup> —Al3—Al4 <sup>iii</sup>	151.28 (3)	Al4 <sup>viii</sup> —Al12—Al2 <sup>i</sup>	60.30 (3)
Al2—Al3—Al4 <sup>iii</sup>	60.55 (2)	Al11—Al12—Al2 <sup>i</sup>	145.56 (3)
Al1—Al3—Al4 <sup>iii</sup>	93.23 (3)	Al13 <sup>xiv</sup> —Al12—Al2 <sup>i</sup>	59.34 (3)
Al5—Al3—Al4 <sup>iii</sup>	57.55 (2)	Cr1 <sup>xv</sup> —Al12—Al2 <sup>i</sup>	53.71 (2)
Al5 <sup>viii</sup> —Al3—Al4 <sup>iii</sup>	107.71 (4)	Al13—Al12—Al14 <sup>xi</sup>	149.04 (4)
Al5 <sup>iv</sup> —Al3—Al4 <sup>iii</sup>	147.76 (4)	Al12 <sup>viii</sup> —Al12—Al14 <sup>xi</sup>	61.237 (17)
Al5 <sup>iii</sup> —Al3—Al4 <sup>iii</sup>	60.95 (2)	Al5 <sup>viii</sup> —Al12—Al14 <sup>xi</sup>	114.16 (3)
C1—Al3—Al4 <sup>iv</sup>	115.75 (18)	Al4 <sup>viii</sup> —Al12—Al14 <sup>xi</sup>	59.15 (3)
Cr2—Al3—Al4 <sup>iv</sup>	57.38 (2)	Al11—Al12—Al14 <sup>xi</sup>	121.93 (3)
Al4—Al3—Al4 <sup>iv</sup>	151.28 (3)	Al13 <sup>xiv</sup> —Al12—Al14 <sup>xi</sup>	59.94 (2)
Al4 <sup>viii</sup> —Al3—Al4 <sup>iv</sup>	90.91 (2)	Cr1 <sup>xv</sup> —Al12—Al14 <sup>xi</sup>	114.06 (3)
Al2—Al3—Al4 <sup>iv</sup>	60.55 (2)	Al2 <sup>i</sup> —Al12—Al14 <sup>xi</sup>	89.99 (3)
Al1—Al3—Al4 <sup>iv</sup>	93.23 (3)	Al13—Al12—Al12 <sup>xiv</sup>	59.70 (3)
Al5—Al3—Al4 <sup>iv</sup>	107.71 (4)	Al12 <sup>viii</sup> —Al12—Al12 <sup>xiv</sup>	90.0
Al5 <sup>viii</sup> —Al3—Al4 <sup>iv</sup>	57.55 (2)	Al5 <sup>viii</sup> —Al12—Al12 <sup>xiv</sup>	153.67 (4)
Al5 <sup>iv</sup> —Al3—Al4 <sup>iv</sup>	60.95 (2)	Al4 <sup>viii</sup> —Al12—Al12 <sup>xiv</sup>	143.19 (4)
Al5 <sup>iii</sup> —Al3—Al4 <sup>iv</sup>	147.76 (4)	Al11—Al12—Al12 <sup>xiv</sup>	89.28 (3)
Al4 <sup>iii</sup> —Al3—Al4 <sup>iv</sup>	108.32 (4)	Al13 <sup>xiv</sup> —Al12—Al12 <sup>xiv</sup>	56.65 (3)
Al16—Cr3—Al13	70.17 (3)	Cr1 <sup>xv</sup> —Al12—Al12 <sup>xiv</sup>	58.779 (15)
Al16—Cr3—Al15	70.90 (3)	Al2 <sup>i</sup> —Al12—Al12 <sup>xiv</sup>	104.77 (3)
Al13—Cr3—Al15	72.84 (2)	Al14 <sup>xi</sup> —Al12—Al12 <sup>xiv</sup>	89.59 (3)
Al16—Cr3—Al19	115.59 (3)	Cr3—Al13—Cr1 <sup>xv</sup>	169.15 (3)
Al13—Cr3—Al19	114.33 (2)	Cr3—Al13—Al12	126.57 (3)
Al15—Cr3—Al19	171.29 (2)	Cr1 <sup>xv</sup> —Al13—Al12	64.26 (2)
Al16—Cr3—Al6 <sup>ix</sup>	115.48 (3)	Cr3—Al13—Al11	64.64 (3)
Al13—Cr3—Al6 <sup>ix</sup>	172.43 (3)	Cr1 <sup>xv</sup> —Al13—Al11	126.19 (3)
Al15—Cr3—Al6 <sup>ix</sup>	113.33 (3)	Al12—Al13—Al11	61.93 (3)
Al19—Cr3—Al6 <sup>ix</sup>	59.13 (2)	Cr3—Al13—Al2 <sup>xv</sup>	114.73 (3)
Al16—Cr3—Cr3 <sup>viii</sup>	173.47 (2)	Cr1 <sup>xv</sup> —Al13—Al2 <sup>xv</sup>	56.69 (2)
Al13—Cr3—Cr3 <sup>viii</sup>	114.464 (19)	Al12—Al13—Al2 <sup>xv</sup>	111.56 (3)
Al15—Cr3—Cr3 <sup>viii</sup>	114.450 (18)	Al11—Al13—Al2 <sup>xv</sup>	150.53 (3)
Al19—Cr3—Cr3 <sup>viii</sup>	58.689 (9)	Cr3—Al13—Al12 <sup>xiv</sup>	120.51 (3)
Al6 <sup>ix</sup> —Cr3—Cr3 <sup>viii</sup>	59.480 (13)	Cr1 <sup>xv</sup> —Al13—Al12 <sup>xiv</sup>	62.92 (2)
Al16—Cr3—Al14	126.40 (3)	Al12—Al13—Al12 <sup>xiv</sup>	63.65 (3)
Al13—Cr3—Al14	66.64 (3)	Al11—Al13—Al12 <sup>xiv</sup>	93.11 (3)
Al15—Cr3—Al14	67.23 (2)	Al2 <sup>xv</sup> —Al13—Al12 <sup>xiv</sup>	60.89 (2)
Al19—Cr3—Al14	110.27 (2)	Cr3—Al13—Al14	60.19 (3)

Al6 <sup>ix</sup> —Cr3—Al14	110.99 (2)	Cr1 <sup>xv</sup> —Al13—Al14	123.42 (3)
Cr3 <sup>viii</sup> —Cr3—Al14	60.097 (13)	Al12—Al13—Al14	94.16 (3)
Al16—Cr3—Al8 <sup>ix</sup>	121.20 (3)	Al11—Al13—Al14	62.05 (3)
Al13—Cr3—Al8 <sup>ix</sup>	122.80 (3)	Al2 <sup>xv</sup> —Al13—Al14	91.33 (3)
Al15—Cr3—Al8 <sup>ix</sup>	62.70 (2)	Al12 <sup>xiv</sup> —Al13—Al14	60.69 (3)
Al9—Cr3—Al8 <sup>ix</sup>	108.60 (2)	Cr3—Al13—Al16	54.85 (2)
Al6 <sup>ix</sup> —Cr3—Al8 <sup>ix</sup>	59.54 (3)	Cr1 <sup>xv</sup> —Al13—Al16	116.06 (3)
Cr3 <sup>viii</sup> —Cr3—Al8 <sup>ix</sup>	60.882 (13)	Al12—Al13—Al16	148.81 (4)
Al14—Cr3—Al8 <sup>ix</sup>	64.12 (3)	Al11—Al13—Al16	109.42 (3)
Al16—Cr3—Al10 <sup>x</sup>	63.14 (3)	Al2 <sup>xv</sup> —Al13—Al16	89.95 (3)
Al13—Cr3—Al10 <sup>x</sup>	118.76 (3)	Al12 <sup>xiv</sup> —Al13—Al16	146.70 (3)
Al15—Cr3—Al10 <sup>x</sup>	121.61 (3)	Al14—Al13—Al16	108.16 (3)
Al9—Cr3—Al10 <sup>x</sup>	60.291 (17)	Cr3—Al13—Al13 <sup>xiii</sup>	114.465 (19)
Al6 <sup>ix</sup> —Cr3—Al10 <sup>x</sup>	62.49 (2)	Cr1 <sup>xv</sup> —Al13—Al13 <sup>xiii</sup>	56.284 (16)
Cr3 <sup>viii</sup> —Cr3—Al10 <sup>x</sup>	110.339 (17)	Al12—Al13—Al13 <sup>xiii</sup>	111.17 (2)
Al14—Cr3—Al10 <sup>x</sup>	170.12 (2)	Al11—Al13—Al13 <sup>xiii</sup>	149.75 (2)
Al8 <sup>ix</sup> —Cr3—Al10 <sup>x</sup>	114.62 (3)	Al2 <sup>xv</sup> —Al13—Al13 <sup>xiii</sup>	59.401 (17)
Al16—Cr3—Al10	66.77 (3)	Al12 <sup>xiv</sup> —Al13—Al13 <sup>xiii</sup>	110.45 (2)
Al13—Cr3—Al10	66.30 (2)	Al14—Al13—Al13 <sup>xiii</sup>	146.32 (2)
Al15—Cr3—Al10	128.53 (3)	Al16—Al13—Al13 <sup>xiii</sup>	59.797 (17)
Al9—Cr3—Al10	60.162 (18)	Cr3—Al13—Al1 <sup>i</sup>	118.16 (3)
Al6 <sup>ix</sup> —Cr3—Al10	110.53 (3)	Cr1 <sup>xv</sup> —Al13—Al1 <sup>i</sup>	63.85 (2)
Cr3 <sup>viii</sup> —Cr3—Al10	110.268 (17)	Al12—Al13—Al1 <sup>i</sup>	64.87 (3)
Al14—Cr3—Al10	118.99 (3)	Al11—Al13—Al1 <sup>i</sup>	92.58 (3)
Al8 <sup>ix</sup> —Cr3—Al10	168.72 (3)	Al2 <sup>xv</sup> —Al13—Al1 <sup>i</sup>	111.01 (3)
Al10 <sup>x</sup> —Cr3—Al10	60.25 (3)	Al12 <sup>xiv</sup> —Al13—Al1 <sup>i</sup>	117.19 (3)
Al16—Cr3—Al7 <sup>x</sup>	66.18 (3)	Al14—Al13—Al1 <sup>i</sup>	153.42 (3)
Al13—Cr3—Al7 <sup>x</sup>	126.51 (3)	Al16—Al13—Al1 <sup>i</sup>	86.80 (3)
Al15—Cr3—Al7 <sup>x</sup>	64.87 (2)	Al13 <sup>xiii</sup> —Al13—Al1 <sup>i</sup>	60.211 (18)
Al9—Cr3—Al7 <sup>x</sup>	111.52 (2)	Cr3—Al13—Al10	61.93 (2)
Al6 <sup>ix</sup> —Cr3—Al7 <sup>x</sup>	61.04 (2)	Cr1 <sup>xv</sup> —Al13—Al10	120.81 (3)
Cr3 <sup>viii</sup> —Cr3—Al7 <sup>x</sup>	112.042 (17)	Al12—Al13—Al10	91.33 (3)
Al14—Cr3—Al7 <sup>x</sup>	119.75 (3)	Al11—Al13—Al10	60.87 (3)
Al8 <sup>ix</sup> —Cr3—Al7 <sup>x</sup>	62.61 (2)	Al2 <sup>xv</sup> —Al13—Al10	147.32 (3)
Al10 <sup>x</sup> —Cr3—Al7 <sup>x</sup>	64.78 (2)	Al12 <sup>xiv</sup> —Al13—Al10	151.16 (3)
Al10—Cr3—Al7 <sup>x</sup>	118.87 (3)	Al14—Al13—Al10	110.64 (3)
Al16—Cr3—Al11	119.60 (3)	Al16—Al13—Al10	60.85 (3)
Al13—Cr3—Al11	62.19 (2)	Al13 <sup>xiii</sup> —Al13—Al10	91.23 (2)
Al15—Cr3—Al11	122.52 (3)	Al1 <sup>i</sup> —Al13—Al10	56.99 (3)
Al9—Cr3—Al11	60.42 (2)	Cr3—Al13—Al15	54.22 (2)
Al6 <sup>ix</sup> —Cr3—Al11	110.24 (2)	Cr1 <sup>xv</sup> —Al13—Al15	117.26 (3)
Cr3 <sup>viii</sup> —Cr3—Al11	61.401 (12)	Al12—Al13—Al15	150.58 (3)
Al14—Cr3—Al11	63.26 (3)	Al11—Al13—Al15	109.59 (3)
Al8 <sup>ix</sup> —Cr3—Al11	115.14 (2)	Al2 <sup>xv</sup> —Al13—Al15	60.66 (3)
Al10 <sup>x</sup> —Cr3—Al11	110.90 (3)	Al12 <sup>xiv</sup> —Al13—Al15	90.17 (3)
Al10—Cr3—Al11	61.49 (2)	Al14—Al13—Al15	59.51 (3)
Al7 <sup>x</sup> —Cr3—Al11	171.19 (3)	Al16—Al13—Al15	59.72 (3)
Al3—Al4—Cr2 <sup>iii</sup>	121.76 (3)	Al13 <sup>xiii</sup> —Al13—Al15	89.680 (19)

Al3—Al4—Al5 <sup>iii</sup>	62.87 (3)	Al1 <sup>i</sup> —Al13—Al15	144.13 (3)
Cr2 <sup>iii</sup> —Al4—Al5 <sup>iii</sup>	59.42 (2)	Al10—Al13—Al15	109.35 (3)
Al3—Al4—Al15 <sup>xi</sup>	153.53 (4)	Cr3 <sup>viii</sup> —Al14—Cr3	59.81 (3)
Cr2 <sup>iii</sup> —Al4—Al15 <sup>xi</sup>	56.47 (2)	Cr3 <sup>viii</sup> —Al14—Al4 <sup>xiv</sup>	111.63 (2)
Al5 <sup>iii</sup> —Al4—Al15 <sup>xi</sup>	105.54 (3)	Cr3—Al14—Al4 <sup>xiv</sup>	150.84 (4)
Al3—Al4—Al14 <sup>xi</sup>	116.65 (3)	Cr3 <sup>viii</sup> —Al14—Al4 <sup>xi</sup>	150.84 (4)
Cr2 <sup>iii</sup> —Al4—Al14 <sup>xi</sup>	118.04 (3)	Cr3—Al14—Al4 <sup>xi</sup>	111.63 (2)
Al5 <sup>iii</sup> —Al4—Al14 <sup>xi</sup>	153.28 (4)	Al4 <sup>xiv</sup> —Al14—Al4 <sup>xi</sup>	60.82 (3)
Al15 <sup>xi</sup> —Al4—Al14 <sup>xi</sup>	62.23 (3)	Cr3 <sup>viii</sup> —Al14—Al13 <sup>viii</sup>	53.171 (19)
Al3—Al4—Al12 <sup>viii</sup>	108.10 (3)	Cr3—Al14—Al13 <sup>viii</sup>	103.32 (3)
Cr2 <sup>iii</sup> —Al4—Al12 <sup>viii</sup>	114.15 (3)	Al4 <sup>xiv</sup> —Al14—Al13 <sup>viii</sup>	88.69 (2)
Al5 <sup>iii</sup> —Al4—Al12 <sup>viii</sup>	145.21 (3)	Al4 <sup>xi</sup> —Al14—Al13 <sup>viii</sup>	145.05 (4)
Al15 <sup>xi</sup> —Al4—Al12 <sup>viii</sup>	94.49 (3)	Cr3 <sup>viii</sup> —Al14—Al13	103.32 (3)
Al14 <sup>xi</sup> —Al4—Al12 <sup>viii</sup>	61.50 (3)	Cr3—Al14—Al13	53.170 (19)
Al3—Al4—Al4 <sup>viii</sup>	57.920 (19)	Al4 <sup>xiv</sup> —Al14—Al13	145.05 (4)
Cr2 <sup>iii</sup> —Al4—Al4 <sup>viii</sup>	152.682 (18)	Al4 <sup>xi</sup> —Al14—Al13	88.69 (2)
Al5 <sup>iii</sup> —Al4—Al4 <sup>viii</sup>	109.27 (2)	Al13 <sup>viii</sup> —Al14—Al13	112.65 (4)
Al15 <sup>xi</sup> —Al4—Al4 <sup>viii</sup>	110.29 (2)	Cr3 <sup>viii</sup> —Al14—Al12 <sup>xiv</sup>	149.13 (4)
Al14 <sup>xi</sup> —Al4—Al4 <sup>viii</sup>	59.591 (18)	Cr3—Al14—Al12 <sup>xiv</sup>	112.24 (2)
Al12 <sup>viii</sup> —Al4—Al4 <sup>viii</sup>	89.22 (2)	Al4 <sup>xiv</sup> —Al14—Al12 <sup>xiv</sup>	88.70 (3)
Al3—Al4—Al2 <sup>iii</sup>	141.08 (4)	Al4 <sup>xi</sup> —Al14—Al12 <sup>xiv</sup>	59.35 (3)
Cr2 <sup>iii</sup> —Al4—Al2 <sup>iii</sup>	53.35 (2)	Al13 <sup>viii</sup> —Al14—Al12 <sup>xiv</sup>	106.95 (4)
Al5 <sup>iii</sup> —Al4—Al2 <sup>iii</sup>	103.69 (3)	Al13—Al14—Al12 <sup>xiv</sup>	59.38 (2)
Al15 <sup>xi</sup> —Al4—Al2 <sup>iii</sup>	62.52 (3)	Cr3 <sup>viii</sup> —Al14—Al12 <sup>xi</sup>	112.24 (2)
Al14 <sup>xi</sup> —Al4—Al2 <sup>iii</sup>	91.63 (3)	Cr3—Al14—Al12 <sup>xi</sup>	149.13 (4)
Al12 <sup>viii</sup> —Al4—Al2 <sup>iii</sup>	60.80 (3)	Al4 <sup>xiv</sup> —Al14—Al12 <sup>xi</sup>	59.35 (3)
Al4 <sup>viii</sup> —Al4—Al2 <sup>iii</sup>	146.87 (2)	Al4 <sup>xi</sup> —Al14—Al12 <sup>xi</sup>	88.70 (3)
Al3—Al4—Al7 <sup>ii</sup>	96.73 (3)	Al13 <sup>viii</sup> —Al14—Al12 <sup>xi</sup>	59.38 (2)
Cr2 <sup>iii</sup> —Al4—Al7 <sup>ii</sup>	62.75 (2)	Al13—Al14—Al12 <sup>xi</sup>	106.95 (4)
Al5 <sup>iii</sup> —Al4—Al7 <sup>ii</sup>	61.96 (2)	Al12 <sup>xiv</sup> —Al14—Al12 <sup>xi</sup>	57.52 (3)
Al15 <sup>xi</sup> —Al4—Al7 <sup>ii</sup>	57.91 (2)	Cr3 <sup>viii</sup> —Al14—Al11	60.26 (3)
Al14 <sup>xi</sup> —Al4—Al7 <sup>ii</sup>	92.57 (3)	Cr3—Al14—Al11	60.26 (3)
Al12 <sup>viii</sup> —Al4—Al7 <sup>ii</sup>	149.96 (3)	Al4 <sup>xiv</sup> —Al14—Al11	143.50 (3)
Al4 <sup>viii</sup> —Al4—Al7 <sup>ii</sup>	89.93 (2)	Al4 <sup>xi</sup> —Al14—Al11	143.50 (3)
Al2 <sup>iii</sup> —Al4—Al7 <sup>ii</sup>	108.79 (3)	Al13 <sup>viii</sup> —Al14—Al11	57.20 (2)
Al3—Al4—Al5	60.42 (3)	Al13—Al14—Al11	57.20 (2)
Cr2 <sup>iii</sup> —Al4—Al5	112.88 (3)	Al12 <sup>xiv</sup> —Al14—Al11	89.46 (3)
Al5 <sup>iii</sup> —Al4—Al5	91.09 (3)	Al12 <sup>xi</sup> —Al14—Al11	89.46 (3)
Al15 <sup>xi</sup> —Al4—Al5	146.01 (3)	Cr3 <sup>viii</sup> —Al14—Al15	103.30 (3)
Al14 <sup>xi</sup> —Al4—Al5	112.22 (3)	Cr3—Al14—Al15	53.621 (19)
Al12 <sup>viii</sup> —Al4—Al5	58.44 (2)	Al4 <sup>xiv</sup> —Al14—Al15	108.43 (4)
Al4 <sup>viii</sup> —Al4—Al5	90.970 (19)	Al4 <sup>xi</sup> —Al14—Al15	58.70 (2)
Al2 <sup>iii</sup> —Al4—Al5	85.05 (3)	Al13 <sup>viii</sup> —Al14—Al15	155.61 (4)
Al7 <sup>ii</sup> —Al4—Al5	151.60 (3)	Al13—Al14—Al15	62.40 (2)
Al3—Al4—Al3 <sup>iii</sup>	89.09 (2)	Al12 <sup>xiv</sup> —Al14—Al15	91.10 (2)
Cr2 <sup>iii</sup> —Al4—Al3 <sup>iii</sup>	55.23 (2)	Al12 <sup>xi</sup> —Al14—Al15	144.45 (3)
Al5 <sup>iii</sup> —Al4—Al3 <sup>iii</sup>	59.20 (3)	Al11—Al14—Al15	108.05 (3)
Al15 <sup>xi</sup> —Al4—Al3 <sup>iii</sup>	105.55 (3)	Cr3 <sup>viii</sup> —Al14—Al15 <sup>viii</sup>	53.621 (19)



Al14 <sup>xi</sup> —Al4—Al3 <sup>iii</sup>	144.52 (3)	Cr3—Al14—Al15 <sup>viii</sup>	103.30 (3)
Al12 <sup>viii</sup> —Al4—Al3 <sup>iii</sup>	88.39 (3)	Al4 <sup>xiv</sup> —Al14—Al15 <sup>viii</sup>	58.70 (2)
Al4 <sup>viii</sup> —Al4—Al3 <sup>iii</sup>	144.16 (2)	Al4 <sup>xi</sup> —Al14—Al15 <sup>viii</sup>	108.43 (4)
Al2 <sup>iii</sup> —Al4—Al3 <sup>iii</sup>	55.35 (3)	Al13 <sup>viii</sup> —Al14—Al15 <sup>viii</sup>	62.40 (2)
Al7 <sup>ii</sup> —Al4—Al3 <sup>iii</sup>	109.09 (3)	Al13—Al14—Al15 <sup>viii</sup>	155.60 (4)
Al5—Al4—Al3 <sup>iii</sup>	57.87 (3)	Al12 <sup>xiv</sup> —Al14—Al15 <sup>viii</sup>	144.45 (3)
C1 <sup>iii</sup> —Al5—Cr2	108.0 (4)	Al12 <sup>xi</sup> —Al14—Al15 <sup>viii</sup>	91.10 (2)
C1 <sup>iii</sup> —Al5—Al6	102.2 (4)	Al11—Al14—Al15 <sup>viii</sup>	108.05 (3)
Cr2—Al5—Al6	55.32 (3)	Al15—Al14—Al15 <sup>viii</sup>	111.28 (4)
C1 <sup>iii</sup> —Al5—Al1 <sup>iii</sup>	41.4 (4)	Cr3 <sup>viii</sup> —Al14—Al8 <sup>ix</sup>	59.05 (3)
Cr2—Al5—Al1 <sup>iii</sup>	148.01 (3)	Cr3—Al14—Al8 <sup>ix</sup>	59.05 (3)
Al6—Al5—Al1 <sup>iii</sup>	113.21 (3)	Al4 <sup>xiv</sup> —Al14—Al8 <sup>ix</sup>	92.19 (3)
C1 <sup>iii</sup> —Al5—Al4 <sup>iii</sup>	67.6 (4)	Al4 <sup>xi</sup> —Al14—Al8 <sup>ix</sup>	92.19 (3)
Cr2—Al5—Al4 <sup>iii</sup>	58.53 (2)	Al13 <sup>viii</sup> —Al14—Al8 <sup>ix</sup>	106.61 (3)
Al6—Al5—Al4 <sup>iii</sup>	104.16 (3)	Al13—Al14—Al8 <sup>ix</sup>	106.61 (3)
Al1 <sup>iii</sup> —Al5—Al4 <sup>iii</sup>	103.44 (3)	Al12 <sup>xiv</sup> —Al14—Al8 <sup>ix</sup>	146.44 (3)
C1 <sup>iii</sup> —Al5—Al12 <sup>viii</sup>	106.6 (4)	Al12 <sup>xi</sup> —Al14—Al8 <sup>ix</sup>	146.44 (3)
Cr2—Al5—Al12 <sup>viii</sup>	145.09 (3)	Al11—Al14—Al8 <sup>ix</sup>	108.70 (4)
Al6—Al5—Al12 <sup>viii</sup>	112.38 (3)	Al15—Al14—Al8 <sup>ix</sup>	56.90 (2)
Al1 <sup>iii</sup> —Al5—Al12 <sup>viii</sup>	65.49 (3)	Al15 <sup>viii</sup> —Al14—Al8 <sup>ix</sup>	56.90 (2)
Al4 <sup>iii</sup> —Al5—Al12 <sup>viii</sup>	143.29 (3)	Cr3—Al15—Cr2 <sup>xv</sup>	162.72 (3)
C1 <sup>iii</sup> —Al5—Al3	128.6 (4)	Cr3—Al15—Al8 <sup>ix</sup>	62.79 (3)
Cr2—Al5—Al3	56.35 (3)	Cr2 <sup>xv</sup> —Al15—Al8 <sup>ix</sup>	132.88 (3)
Al6—Al5—Al3	103.18 (3)	Cr3—Al15—Al7 <sup>xvi</sup>	129.66 (3)
Al1 <sup>iii</sup> —Al5—Al3	143.48 (4)	Cr2 <sup>xv</sup> —Al15—Al7 <sup>xvi</sup>	66.04 (2)
Al4 <sup>iii</sup> —Al5—Al3	63.25 (3)	Al8 <sup>ix</sup> —Al15—Al7 <sup>xvi</sup>	67.00 (3)
Al12 <sup>viii</sup> —Al5—Al3	103.79 (3)	Cr3—Al15—Al4 <sup>xi</sup>	117.44 (3)
C1 <sup>iii</sup> —Al5—Al3 <sup>iii</sup>	51.8 (4)	Cr2 <sup>xv</sup> —Al15—Al4 <sup>xi</sup>	59.70 (2)
Cr2—Al5—Al3 <sup>iii</sup>	114.74 (3)	Al8 <sup>ix</sup> —Al15—Al4 <sup>xi</sup>	95.44 (3)
Al6—Al5—Al3 <sup>iii</sup>	150.74 (4)	Al7 <sup>xvi</sup> —Al15—Al4 <sup>xi</sup>	63.33 (3)
Al1 <sup>iii</sup> —Al5—Al3 <sup>iii</sup>	58.61 (3)	Cr3—Al15—Al8 <sup>xv</sup>	126.60 (3)
Al4 <sup>iii</sup> —Al5—Al3 <sup>iii</sup>	56.67 (3)	Cr2 <sup>xv</sup> —Al15—Al8 <sup>xv</sup>	64.47 (3)
Al12 <sup>viii</sup> —Al5—Al3 <sup>iii</sup>	90.41 (3)	Al8 <sup>ix</sup> —Al15—Al8 <sup>xv</sup>	96.52 (2)
Al3—Al5—Al3 <sup>iii</sup>	88.00 (2)	Al7 <sup>xvi</sup> —Al15—Al8 <sup>xv</sup>	62.03 (3)
C1 <sup>iii</sup> —Al5—Al7 <sup>viii</sup>	51.2 (4)	Al4 <sup>xi</sup> —Al15—Al8 <sup>xv</sup>	112.89 (3)
Cr2—Al5—Al7 <sup>viii</sup>	62.22 (2)	Cr3—Al15—Al15 <sup>xii</sup>	114.451 (18)
Al6—Al5—Al7 <sup>viii</sup>	58.16 (2)	Cr2 <sup>xv</sup> —Al15—Al15 <sup>xii</sup>	56.841 (17)
Al1 <sup>iii</sup> —Al5—Al7 <sup>viii</sup>	86.15 (3)	Al8 <sup>ix</sup> —Al15—Al15 <sup>xii</sup>	150.02 (2)
Al4 <sup>iii</sup> —Al5—Al7 <sup>viii</sup>	61.30 (2)	Al7 <sup>xvi</sup> —Al15—Al15 <sup>xii</sup>	110.55 (2)
Al12 <sup>viii</sup> —Al5—Al7 <sup>viii</sup>	144.42 (3)	Al4 <sup>xi</sup> —Al15—Al15 <sup>xii</sup>	110.29 (2)
Al3—Al5—Al7 <sup>viii</sup>	111.74 (3)	Al8 <sup>xv</sup> —Al15—Al15 <sup>xii</sup>	59.907 (18)
Al3 <sup>iii</sup> —Al5—Al7 <sup>viii</sup>	92.60 (3)	Cr3—Al15—Al7 <sup>x</sup>	62.10 (2)
C1 <sup>iii</sup> —Al5—Al5 <sup>viii</sup>	159.0 (4)	Cr2 <sup>xv</sup> —Al15—Al7 <sup>x</sup>	128.46 (3)
Cr2—Al5—Al5 <sup>viii</sup>	57.205 (17)	Al8 <sup>ix</sup> —Al15—Al7 <sup>x</sup>	61.76 (3)
Al6—Al5—Al5 <sup>viii</sup>	57.562 (19)	Al7 <sup>xvi</sup> —Al15—Al7 <sup>x</sup>	97.30 (3)
Al1 <sup>iii</sup> —Al5—Al5 <sup>viii</sup>	147.27 (2)	Al4 <sup>xi</sup> —Al15—Al7 <sup>x</sup>	155.52 (3)
Al4 <sup>iii</sup> —Al5—Al5 <sup>viii</sup>	109.27 (2)	Al8 <sup>xv</sup> —Al15—Al7 <sup>x</sup>	64.78 (3)
Al12 <sup>viii</sup> —Al5—Al5 <sup>viii</sup>	88.21 (2)	Al15 <sup>xii</sup> —Al15—Al7 <sup>x</sup>	89.94 (2)

Al3—Al5—Al5 <sup>viii</sup>	58.761 (18)	Cr3—Al15—Al14	59.14 (3)
Al3 <sup>iii</sup> —Al5—Al5 <sup>viii</sup>	145.21 (2)	Cr2 <sup>xv</sup> —Al15—Al14	118.11 (3)
Al7 <sup>viii</sup> —Al5—Al5 <sup>viii</sup>	108.29 (2)	Al8 <sup>ix</sup> —Al15—Al14	61.58 (3)
C1 <sup>iii</sup> —Al5—Al4	111.4 (4)	Al7 <sup>xvi</sup> —Al15—Al14	93.91 (3)
Cr2—Al5—Al4	111.45 (3)	Al4 <sup>xi</sup> —Al15—Al14	59.07 (3)
Al6—Al5—Al4	146.44 (3)	Al8 <sup>xv</sup> —Al15—Al14	153.46 (3)
Al1 <sup>iii</sup> —Al5—Al4	92.87 (3)	Al15 <sup>xii</sup> —Al15—Al14	145.64 (2)
Al4 <sup>iii</sup> —Al5—Al4	88.91 (3)	Al7 <sup>x</sup> —Al15—Al14	111.13 (3)
Al12 <sup>viii</sup> —Al5—Al4	58.49 (2)	Cr3—Al15—Al16	53.826 (19)
Al3—Al5—Al4	55.14 (3)	Cr2 <sup>xv</sup> —Al15—Al16	116.32 (3)
Al3 <sup>iii</sup> —Al5—Al4	61.18 (3)	Al8 <sup>ix</sup> —Al15—Al16	107.54 (3)
Al7 <sup>viii</sup> —Al5—Al4	148.87 (3)	Al7 <sup>xvi</sup> —Al15—Al16	154.16 (4)
Al5 <sup>viii</sup> —Al5—Al4	89.031 (19)	Al4 <sup>xi</sup> —Al15—Al16	141.72 (3)
Cr2—Al6—Al9	178.55 (4)	Al8 <sup>xv</sup> —Al15—Al16	94.83 (3)
Cr2—Al6—Cr3 <sup>ix</sup>	119.55 (3)	Al15 <sup>xii</sup> —Al15—Al16	60.744 (17)
Al9—Al6—Cr3 <sup>ix</sup>	59.27 (2)	Al7 <sup>x</sup> —Al15—Al16	60.20 (3)
Cr2—Al6—Cr3 <sup>x</sup>	119.55 (3)	Al14—Al15—Al16	105.66 (3)
Al9—Al6—Cr3 <sup>x</sup>	59.27 (2)	Cr3—Al15—Al2 <sup>xv</sup>	109.88 (3)
Cr3 <sup>ix</sup> —Al6—Cr3 <sup>x</sup>	61.04 (3)	Cr2 <sup>xv</sup> —Al15—Al2 <sup>xv</sup>	53.18 (2)
Cr2—Al6—Al8	67.50 (3)	Al8 <sup>ix</sup> —Al15—Al2 <sup>xv</sup>	148.91 (3)
Al9—Al6—Al8	111.05 (4)	Al7 <sup>xvi</sup> —Al15—Al2 <sup>xv</sup>	110.84 (3)
Cr3 <sup>ix</sup> —Al6—Al8	62.37 (3)	Al4 <sup>xi</sup> —Al15—Al2 <sup>xv</sup>	59.70 (2)
Cr3 <sup>x</sup> —Al6—Al8	62.37 (3)	Al8 <sup>xv</sup> —Al15—Al2 <sup>xv</sup>	109.86 (3)
Cr2—Al6—Al5	61.81 (3)	Al15 <sup>xii</sup> —Al15—Al2 <sup>xv</sup>	61.023 (17)
Al9—Al6—Al5	119.34 (3)	Al7 <sup>x</sup> —Al15—Al2 <sup>xv</sup>	144.77 (3)
Cr3 <sup>ix</sup> —Al6—Al5	117.04 (2)	Al14—Al15—Al2 <sup>xv</sup>	88.31 (3)
Cr3 <sup>x</sup> —Al6—Al5	177.94 (3)	Al16—Al15—Al2 <sup>xv</sup>	86.87 (3)
Al8—Al6—Al5	117.73 (4)	Cr3—Al15—Al13	52.94 (2)
Cr2—Al6—Al5 <sup>viii</sup>	61.81 (3)	Cr2 <sup>xv</sup> —Al15—Al13	110.25 (3)
Al9—Al6—Al5 <sup>viii</sup>	119.34 (3)	Al8 <sup>ix</sup> —Al15—Al13	106.88 (3)
Cr3 <sup>ix</sup> —Al6—Al5 <sup>viii</sup>	177.94 (3)	Al7 <sup>xvi</sup> —Al15—Al13	147.44 (3)
Cr3 <sup>x</sup> —Al6—Al5 <sup>viii</sup>	117.035 (19)	Al4 <sup>xi</sup> —Al15—Al13	86.44 (3)
Al8—Al6—Al5 <sup>viii</sup>	117.73 (4)	Al8 <sup>xv</sup> —Al15—Al13	148.22 (3)
Al5—Al6—Al5 <sup>viii</sup>	64.88 (4)	Al15 <sup>xii</sup> —Al15—Al13	90.319 (19)
Cr2—Al6—Al7 <sup>viii</sup>	66.91 (2)	Al7 <sup>x</sup> —Al15—Al13	107.77 (3)
Al9—Al6—Al7 <sup>viii</sup>	112.59 (2)	Al14—Al15—Al13	58.09 (3)
Cr3 <sup>ix</sup> —Al6—Al7 <sup>viii</sup>	62.16 (2)	Al16—Al15—Al13	58.07 (3)
Cr3 <sup>x</sup> —Al6—Al7 <sup>viii</sup>	114.30 (3)	Al2 <sup>xv</sup> —Al15—Al13	57.07 (2)
Al8—Al6—Al7 <sup>viii</sup>	63.93 (2)	Cr3 <sup>xii</sup> —Al16—Cr3	166.95 (5)
Al5—Al6—Al7 <sup>viii</sup>	64.52 (2)	Cr3 <sup>xii</sup> —Al16—Al10 <sup>x</sup>	129.30 (4)
Al5 <sup>viii</sup> —Al6—Al7 <sup>viii</sup>	119.85 (4)	Cr3—Al16—Al10 <sup>x</sup>	63.74 (2)
Cr2—Al6—Al7	66.91 (2)	Cr3 <sup>xii</sup> —Al16—Al10 <sup>xiii</sup>	63.74 (2)
Al9—Al6—Al7	112.59 (2)	Cr3—Al16—Al10 <sup>xiii</sup>	129.30 (4)
Cr3 <sup>ix</sup> —Al6—Al7	114.30 (3)	Al10 <sup>x</sup> —Al16—Al10 <sup>xiii</sup>	65.56 (4)
Cr3 <sup>x</sup> —Al6—Al7	62.16 (2)	Cr3 <sup>xii</sup> —Al16—Al13	115.20 (4)
Al8—Al6—Al7	63.93 (2)	Cr3—Al16—Al13	54.98 (2)
Al5—Al6—Al7	119.85 (4)	Al10 <sup>x</sup> —Al16—Al13	107.53 (3)
Al5 <sup>viii</sup> —Al6—Al7	64.52 (2)	Al10 <sup>xiii</sup> —Al16—Al13	147.77 (4)

Al7 <sup>viii</sup> —Al6—Al7	119.74 (4)	Cr3 <sup>xii</sup> —Al16—Al13 <sup>xii</sup>	54.98 (2)
Cr2—Al6—Al10 <sup>viii</sup>	120.60 (2)	Cr3—Al16—Al13 <sup>xii</sup>	115.20 (4)
Al9—Al6—Al10 <sup>viii</sup>	59.85 (2)	Al10 <sup>x</sup> —Al16—Al13 <sup>xii</sup>	147.77 (4)
Cr3 <sup>ix</sup> —Al6—Al10 <sup>viii</sup>	61.15 (2)	Al10 <sup>xiii</sup> —Al16—Al13 <sup>xii</sup>	107.53 (3)
Cr3 <sup>x</sup> —Al6—Al10 <sup>viii</sup>	110.50 (3)	Al13—Al16—Al13 <sup>xii</sup>	60.41 (3)
Al8—Al6—Al10 <sup>viii</sup>	115.89 (3)	Cr3 <sup>xii</sup> —Al16—Al7 <sup>x</sup>	120.36 (4)
Al5—Al6—Al10 <sup>viii</sup>	67.52 (2)	Cr3—Al16—Al7 <sup>x</sup>	62.11 (2)
Al5 <sup>viii</sup> —Al6—Al10 <sup>viii</sup>	119.82 (4)	Al10 <sup>x</sup> —Al16—Al7 <sup>x</sup>	63.66 (3)
Al7 <sup>viii</sup> —Al6—Al10 <sup>viii</sup>	64.69 (2)	Al10 <sup>xiii</sup> —Al16—Al7 <sup>x</sup>	94.97 (4)
Al7—Al6—Al10 <sup>viii</sup>	172.24 (4)	Al13—Al16—Al7 <sup>x</sup>	110.32 (3)
Cr2—Al6—Al10	120.60 (2)	Al13 <sup>xii</sup> —Al16—Al7 <sup>x</sup>	147.13 (4)
Al9—Al6—Al10	59.85 (2)	Cr3 <sup>xii</sup> —Al16—Al7 <sup>xiii</sup>	62.11 (2)
Cr3 <sup>ix</sup> —Al6—Al10	110.50 (3)	Cr3—Al16—Al7 <sup>xiii</sup>	120.36 (4)
Cr3 <sup>x</sup> —Al6—Al10	61.15 (2)	Al10 <sup>x</sup> —Al16—Al7 <sup>xiii</sup>	94.97 (4)
Al8—Al6—Al10	115.89 (3)	Al10 <sup>xiii</sup> —Al16—Al7 <sup>xiii</sup>	63.66 (3)
Al5—Al6—Al10	119.82 (4)	Al13—Al16—Al7 <sup>xiii</sup>	147.13 (4)
Al5 <sup>viii</sup> —Al6—Al10	67.52 (2)	Al13 <sup>xii</sup> —Al16—Al7 <sup>xiii</sup>	110.32 (3)
Al7 <sup>viii</sup> —Al6—Al10	172.24 (4)	Al7 <sup>x</sup> —Al16—Al7 <sup>xiii</sup>	58.65 (4)
Al7—Al6—Al10	64.69 (2)	Cr3 <sup>xii</sup> —Al16—Al15 <sup>xii</sup>	55.27 (2)
Al10 <sup>viii</sup> —Al6—Al10	110.15 (4)	Cr3—Al16—Al15 <sup>xii</sup>	113.67 (3)
Cr2—Al6—Al11	121.55 (4)	Al10 <sup>x</sup> —Al16—Al15 <sup>xii</sup>	149.83 (4)
Al9—Al6—Al11	59.90 (3)	Al10 <sup>xiii</sup> —Al16—Al15 <sup>xii</sup>	109.59 (3)
Cr3 <sup>ix</sup> —Al6—Al11	110.11 (3)	Al13—Al16—Al15 <sup>xii</sup>	91.46 (3)
Cr3 <sup>x</sup> —Al6—Al11	110.11 (3)	Al13 <sup>xii</sup> —Al16—Al15 <sup>xii</sup>	62.21 (3)
Al8—Al6—Al11	170.95 (5)	Al7 <sup>x</sup> —Al16—Al15 <sup>xii</sup>	88.07 (3)
Al5—Al6—Al11	69.59 (3)	Al7 <sup>xiii</sup> —Al16—Al15 <sup>xii</sup>	59.18 (3)
Al5 <sup>viii</sup> —Al6—Al11	69.59 (3)	Cr3 <sup>xii</sup> —Al16—Al15	113.67 (3)
Al7 <sup>viii</sup> —Al6—Al11	118.17 (2)	Cr3—Al16—Al15	55.27 (2)
Al7—Al6—Al11	118.17 (2)	Al10 <sup>x</sup> —Al16—Al15	109.59 (3)
Al10 <sup>viii</sup> —Al6—Al11	60.69 (2)	Al10 <sup>xiii</sup> —Al16—Al15	149.83 (4)
Al10—Al6—Al11	60.69 (2)	Al13—Al16—Al15	62.21 (3)
C1 <sup>i</sup> —Al7—Al6	104.7 (3)	Al13 <sup>xii</sup> —Al16—Al15	91.46 (3)
C1 <sup>i</sup> —Al7—Al15 <sup>vii</sup>	123.3 (4)	Al7 <sup>x</sup> —Al16—Al15	59.18 (3)
Al6—Al7—Al15 <sup>vii</sup>	98.86 (3)	Al7 <sup>xiii</sup> —Al16—Al15	88.07 (3)
C1 <sup>i</sup> —Al7—Cr3 <sup>x</sup>	119.6 (4)	Al15 <sup>xii</sup> —Al16—Al15	58.51 (3)
Al6—Al7—Cr3 <sup>x</sup>	56.80 (2)	Cr3 <sup>xii</sup> —Al16—Al10	123.24 (4)
Al15 <sup>vii</sup> —Al7—Cr3 <sup>x</sup>	116.53 (3)	Cr3—Al16—Al10	61.71 (2)
C1 <sup>i</sup> —Al7—Al7 <sup>xii</sup>	53.6 (2)	Al10 <sup>x</sup> —Al16—Al10	58.93 (3)
Al6—Al7—Al7 <sup>xii</sup>	149.87 (2)	Al10 <sup>xiii</sup> —Al16—Al10	92.35 (3)
Al15 <sup>vii</sup> —Al7—Al7 <sup>xii</sup>	110.56 (2)	Al13—Al16—Al10	60.28 (2)
Cr3 <sup>x</sup> —Al7—Al7 <sup>xii</sup>	112.042 (17)	Al13 <sup>xii</sup> —Al16—Al10	91.25 (3)
C1 <sup>i</sup> —Al7—Al15 <sup>x</sup>	139.6 (3)	Al7 <sup>x</sup> —Al16—Al10	111.89 (3)
Al6—Al7—Al15 <sup>x</sup>	100.28 (3)	Al7 <sup>xiii</sup> —Al16—Al10	151.23 (4)
Al15 <sup>vii</sup> —Al7—Al15 <sup>x</sup>	82.70 (3)	Al15 <sup>xii</sup> —Al16—Al10	149.25 (4)
Cr3 <sup>x</sup> —Al7—Al15 <sup>x</sup>	53.03 (2)	Al15—Al16—Al10	110.90 (3)
Al7 <sup>xii</sup> —Al7—Al15 <sup>x</sup>	90.06 (2)	Cr3 <sup>xii</sup> —Al16—Al10 <sup>xii</sup>	61.71 (2)
C1 <sup>i</sup> —Al7—Al8	160.3 (2)	Cr3—Al16—Al10 <sup>xii</sup>	123.24 (4)
Al6—Al7—Al8	56.68 (3)	Al10 <sup>x</sup> —Al16—Al10 <sup>xii</sup>	92.35 (3)

Al15 <sup>vii</sup> —Al7—Al8	60.04 (3)	Al10 <sup>xiii</sup> —Al16—Al10 <sup>xii</sup>	58.93 (3)
Cr3 <sup>x</sup> —Al7—Al8	58.11 (3)	Al13—Al16—Al10 <sup>xii</sup>	91.25 (3)
Al7 <sup>xii</sup> —Al7—Al8	145.96 (2)	Al13 <sup>xii</sup> —Al16—Al10 <sup>xii</sup>	60.29 (2)
Al15 <sup>x</sup> —Al7—Al8	57.33 (3)	Al7 <sup>x</sup> —Al16—Al10 <sup>xii</sup>	151.23 (4)
C1 <sup>i</sup> —Al7—Al16 <sup>xiii</sup>	83.9 (4)	Al7 <sup>xiii</sup> —Al16—Al10 <sup>xii</sup>	111.89 (3)
Al6—Al7—Al16 <sup>xiii</sup>	100.02 (3)	Al15 <sup>xii</sup> —Al16—Al10 <sup>xii</sup>	110.90 (3)
Al15 <sup>vii</sup> —Al7—Al16 <sup>xiii</sup>	141.08 (4)	Al15—Al16—Al10 <sup>xii</sup>	149.25 (4)
Cr3 <sup>x</sup> —Al7—Al16 <sup>xiii</sup>	51.703 (18)	Al10—Al16—Al10 <sup>xii</sup>	61.91 (3)
Al7 <sup>xii</sup> —Al7—Al16 <sup>xiii</sup>	60.678 (18)		

Symmetry codes: (i)  $-x+1/2, -y+1/2, -z+1$ ; (ii)  $-x+1/2, y+1/2, -z+1$ ; (iii)  $-x+1/2, -y+3/2, -z+1$ ; (iv)  $-x+1/2, y-1/2, -z+1$ ; (v)  $-x, -y+1, -z+1$ ; (vi)  $x-1/2, y+1/2, z$ ; (vii)  $x-1/2, -y+1/2, z$ ; (viii)  $x, -y+1, z$ ; (ix)  $-x+1, -y+1, -z+2$ ; (x)  $-x+1, y, -z+2$ ; (xi)  $-x+1, -y+1, -z+1$ ; (xii)  $x, -y, z$ ; (xiii)  $-x+1, -y, -z+2$ ; (xiv)  $-x+1, y, -z+1$ ; (xv)  $x+1/2, y-1/2, z$ ; (xvi)  $x+1/2, -y+1/2, z$ .